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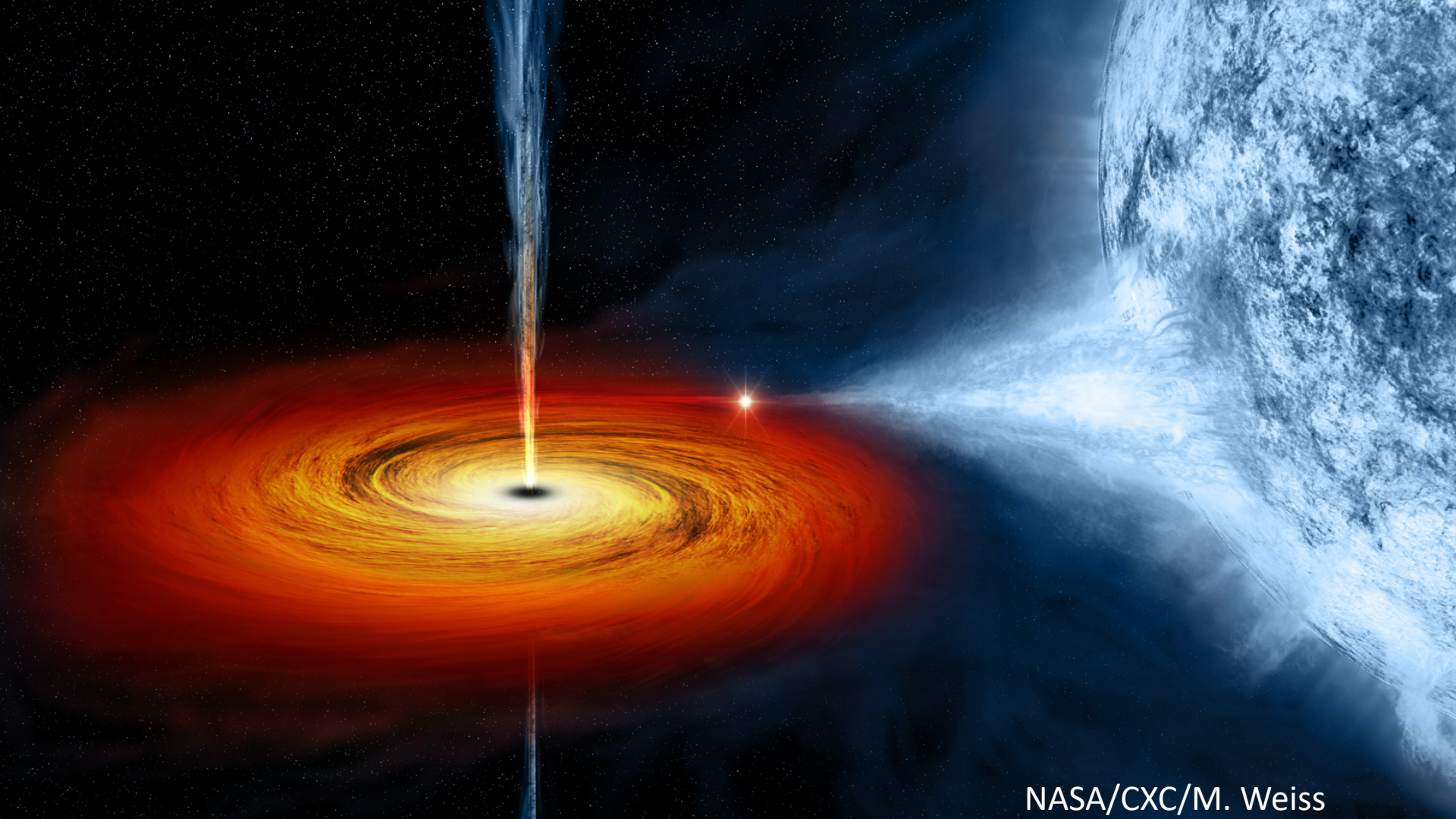
Black Holes: Connecting Theory and Simulation to Observation

Brooks E. Kinch

Los Alamos National Laboratory, Metropolis Fellow, CCS-2

Lawrence Livermore National Laboratory

2/17/2021



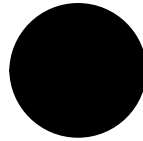
NASA/CXC/M. Weiss

Agenda:

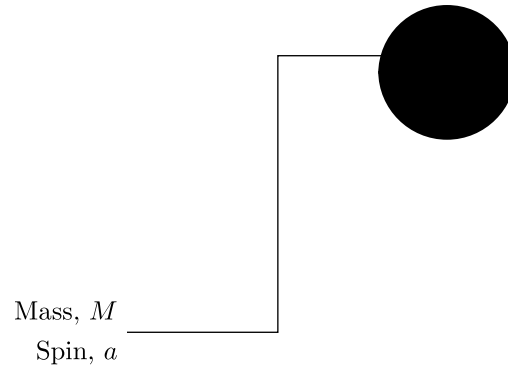
- Review the relevant basics of black holes and black hole astrophysics.
- Discuss the underlying principles and methodology behind simulating infalling plasma, along with recent advances.
- Show how we generate synthetic X-ray spectra starting from simulation data.
- Connect these X-ray spectra to real observations.

- What are the current challenges facing this technique, and how might they be resolved?



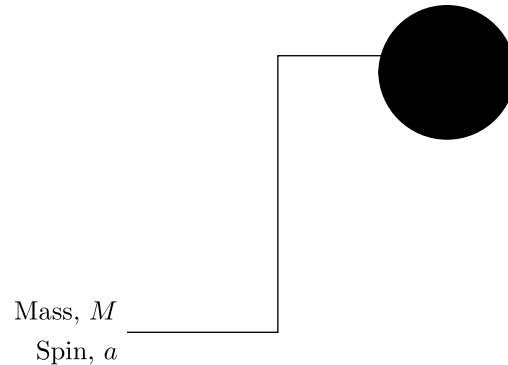


Black holes are characterized entirely by only two parameters:
mass and dimensionless “spin.”



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$$-1 < a = \frac{J}{GM^2/c} < +1$$



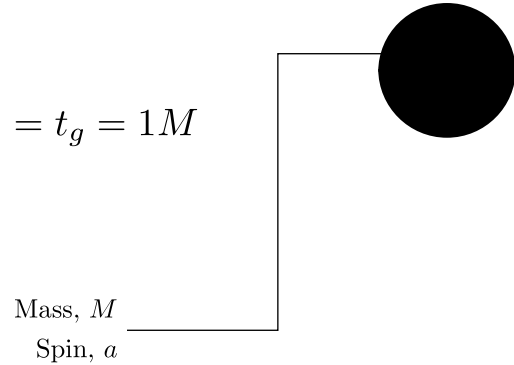
The central black hole mass sets the *length* and *time* scales for the whole system.

$$r_g = \frac{GM}{c^2} = \left(\frac{M}{M_\odot} \right) \cdot 1.5 \times 10^5 \text{ cm}$$

$$t_g = r_g/c = \left(\frac{M}{M_\odot} \right) \cdot 4.9 \times 10^{-6} \text{ s}$$

$$G = c = 1 \rightarrow r_g = t_g = 1M$$

Mass, M
Spin, a



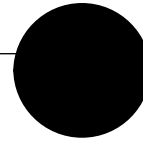
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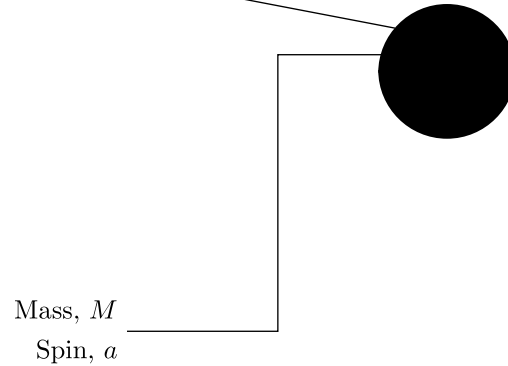


Light travels 1M (distance) in 1M (time).



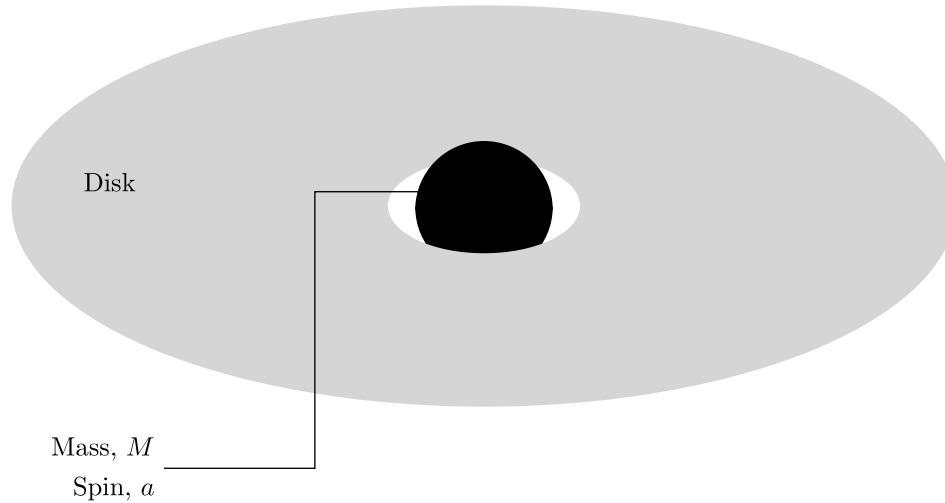
The radius of the event horizon decreases with increasing spin.

$$r_h/M = 1 + \sqrt{1 - a^2}$$



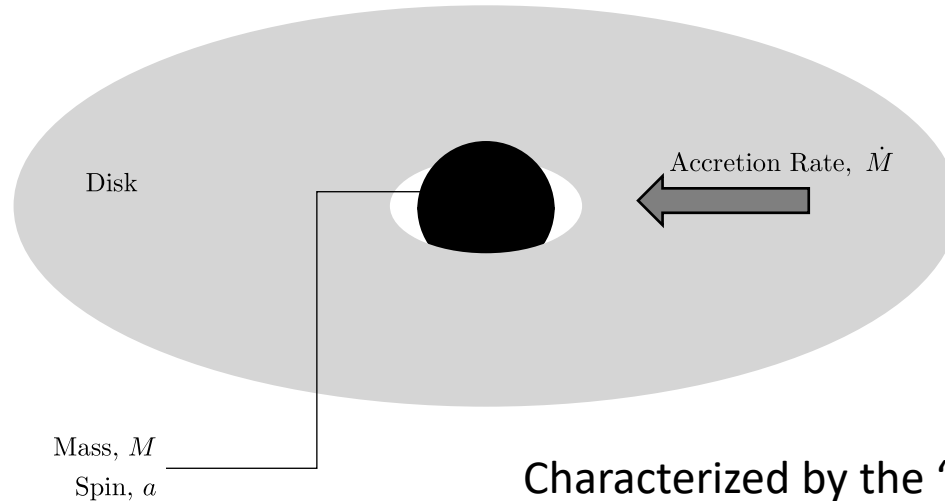
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but conserves angular momentum.

black hole basics



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Result: a geometrically thin, optically thick, slowly spiraling inward accretion disk.

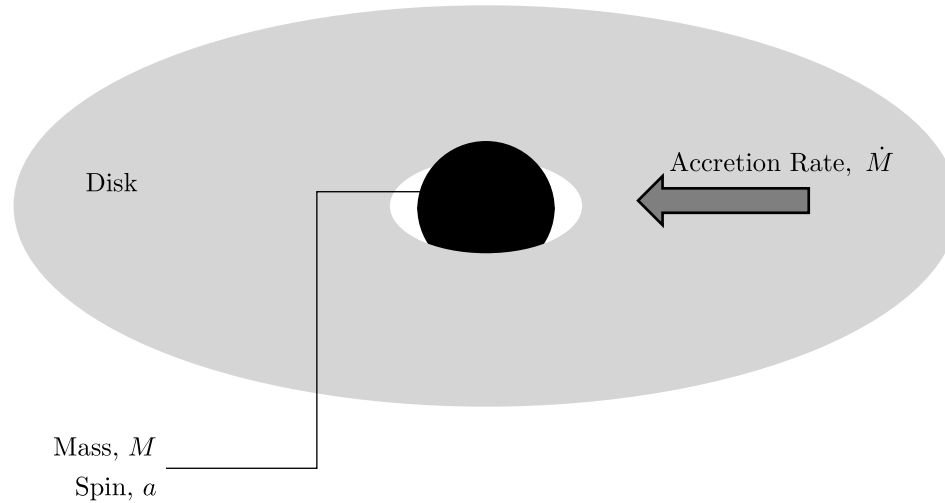


Characterized by the “accretion rate”:
inward mass flow rate per unit time.



The black hole mass sets the characteristic
“Eddington” *luminosity* and *accretion rate*.

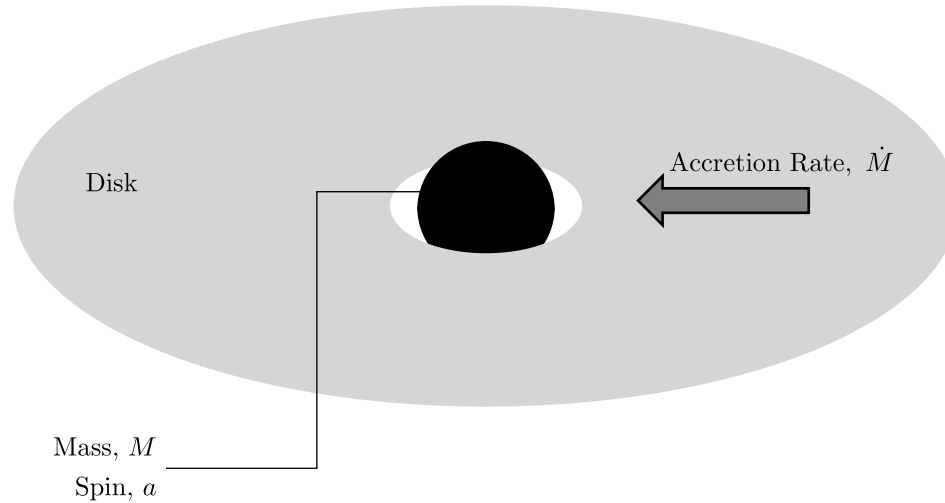
$$L_{\text{Edd}} = \frac{4\pi GMm_p c}{\sigma_T} = \left(\frac{M}{M_{\odot}} \right) \cdot 1.3 \times 10^{38} \text{ erg s}^{-1} = \eta \dot{M}_{\text{Edd}} c^2$$



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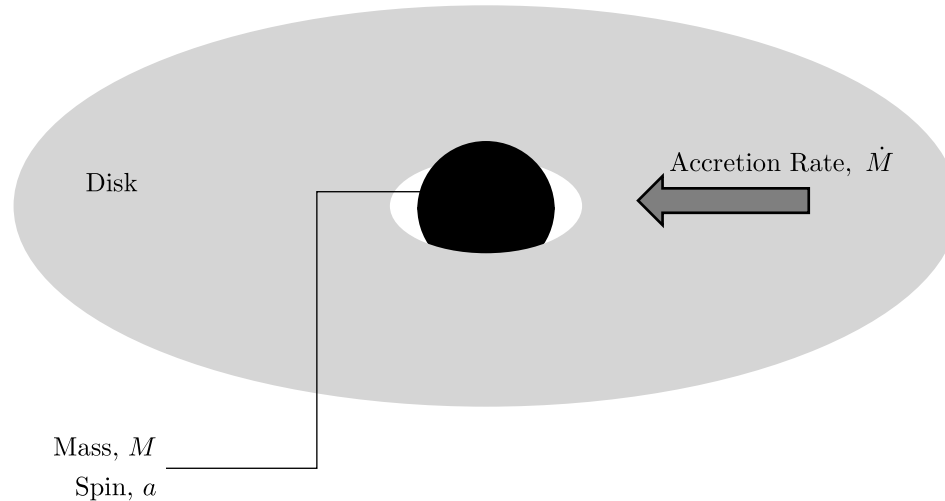


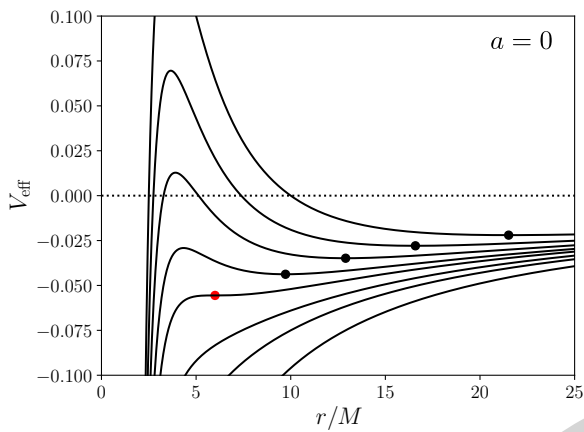
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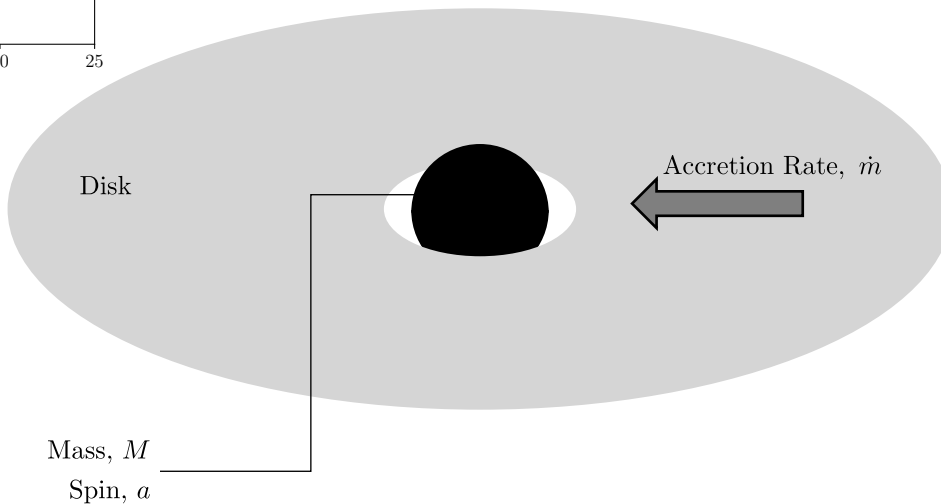
$$\dot{m} = \frac{\dot{M}}{\dot{M}_{\text{Edd}}}$$



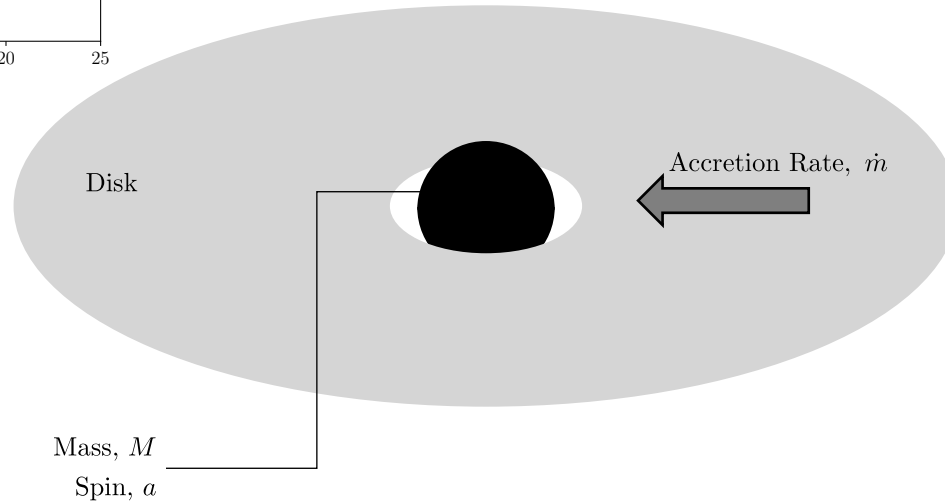
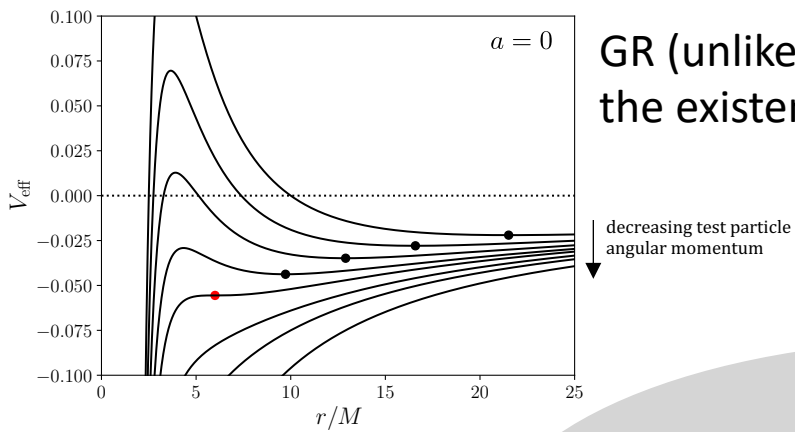


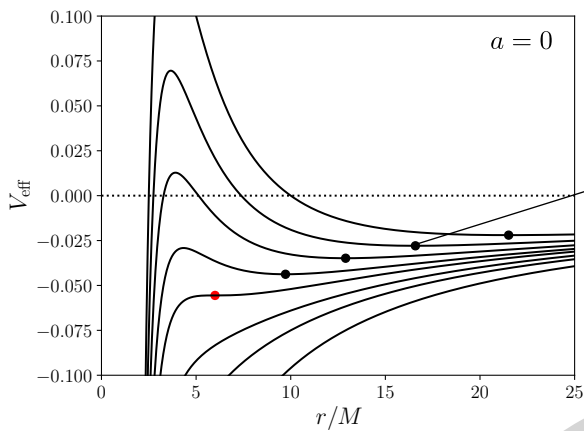
GR (unlike Newtonian gravity) constrains the existence of circular orbits.

black hole basics

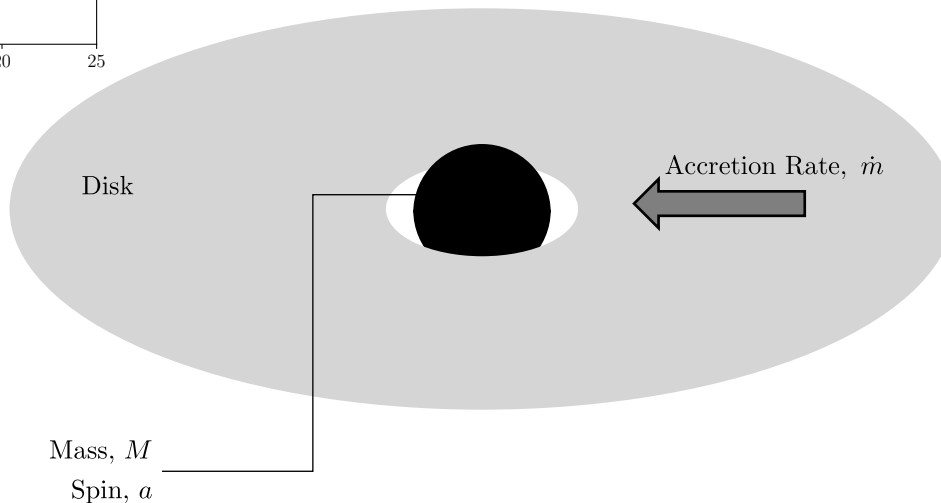


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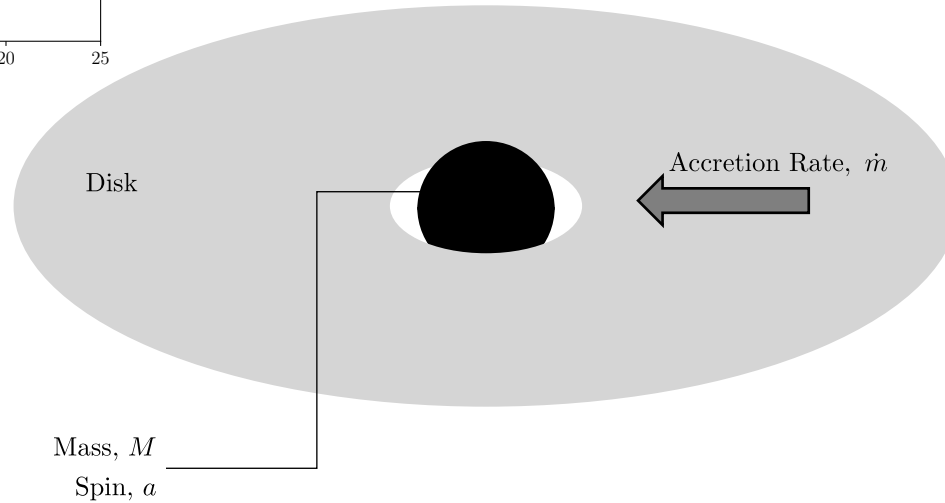
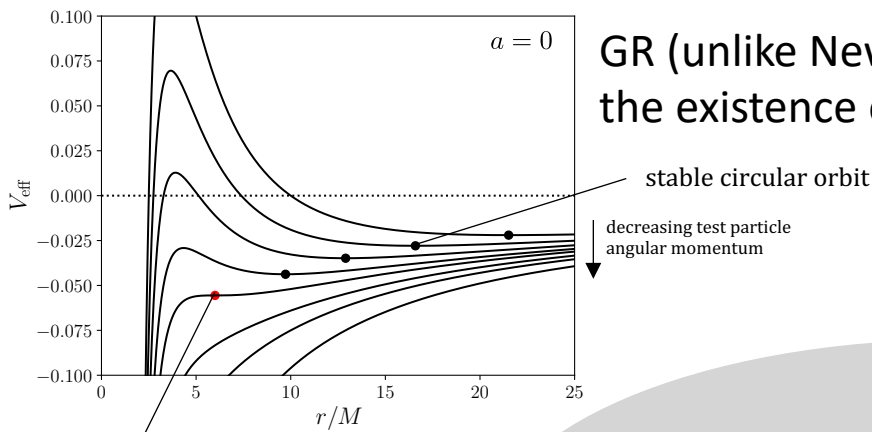




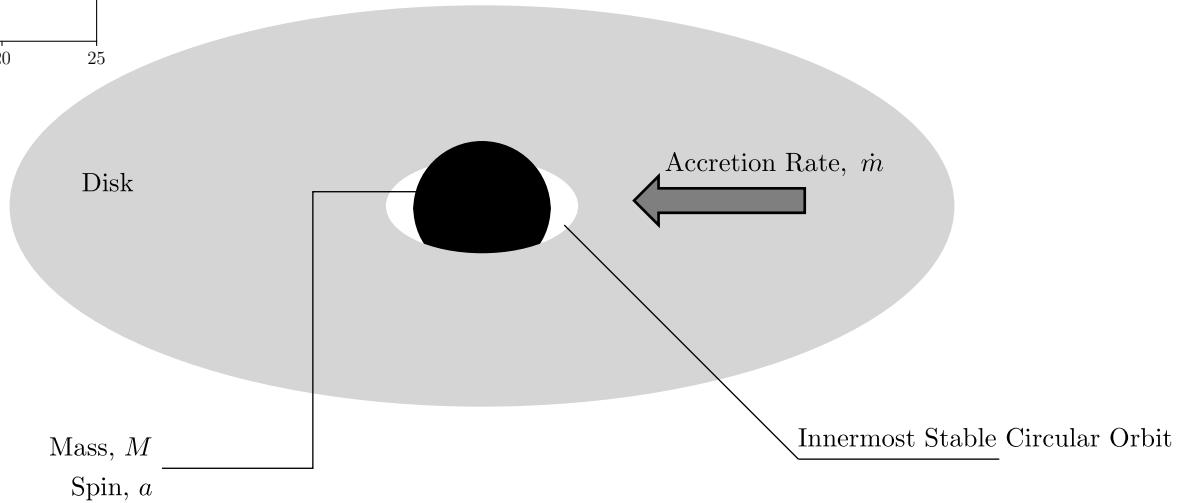
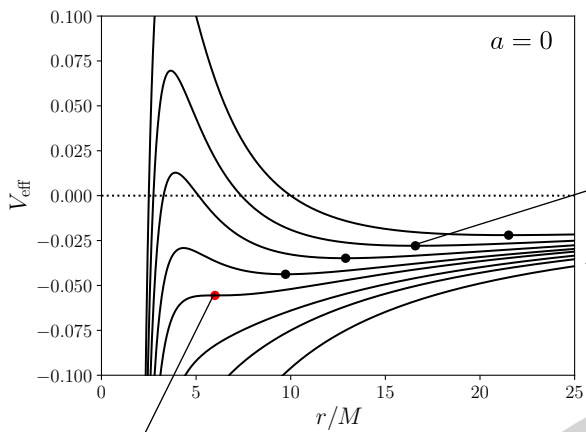
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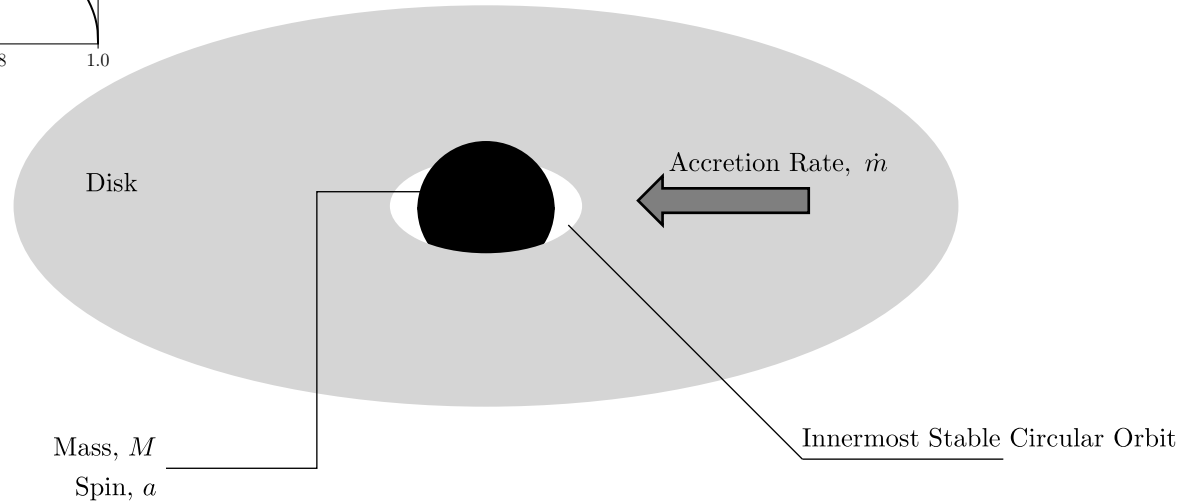
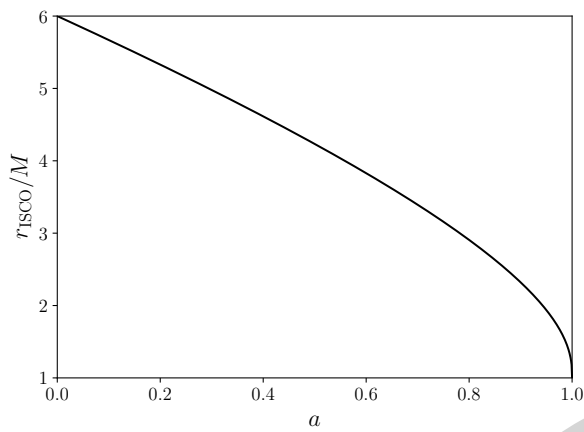


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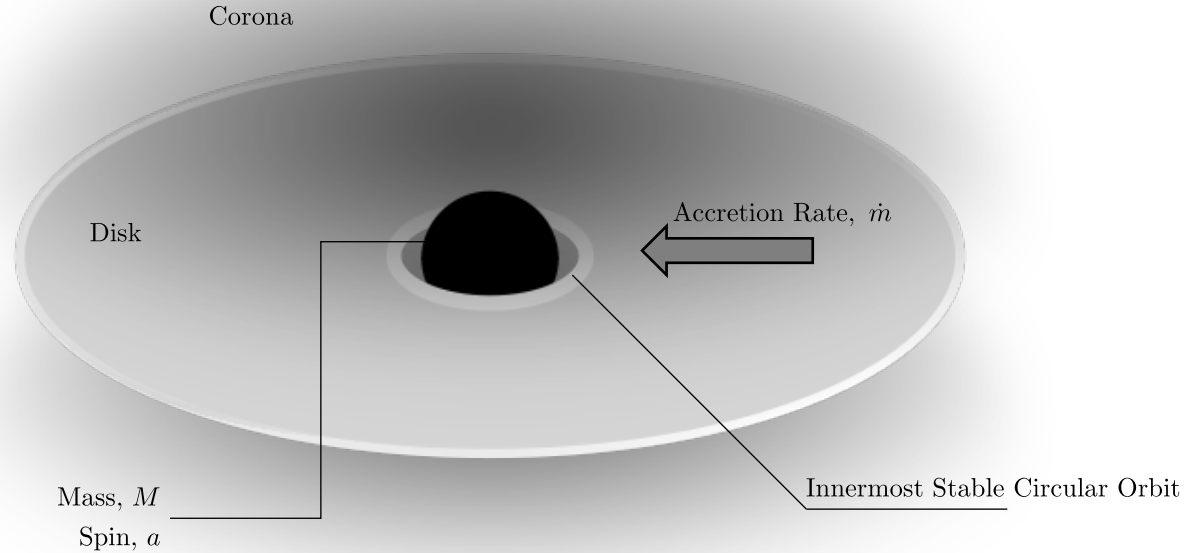
black hole basics

ISCO radius (like event horizon radius)
decreases with increasing spin.



Above and below the dense cool disk lies
the magnetically-supported, hot, diffuse *corona*.

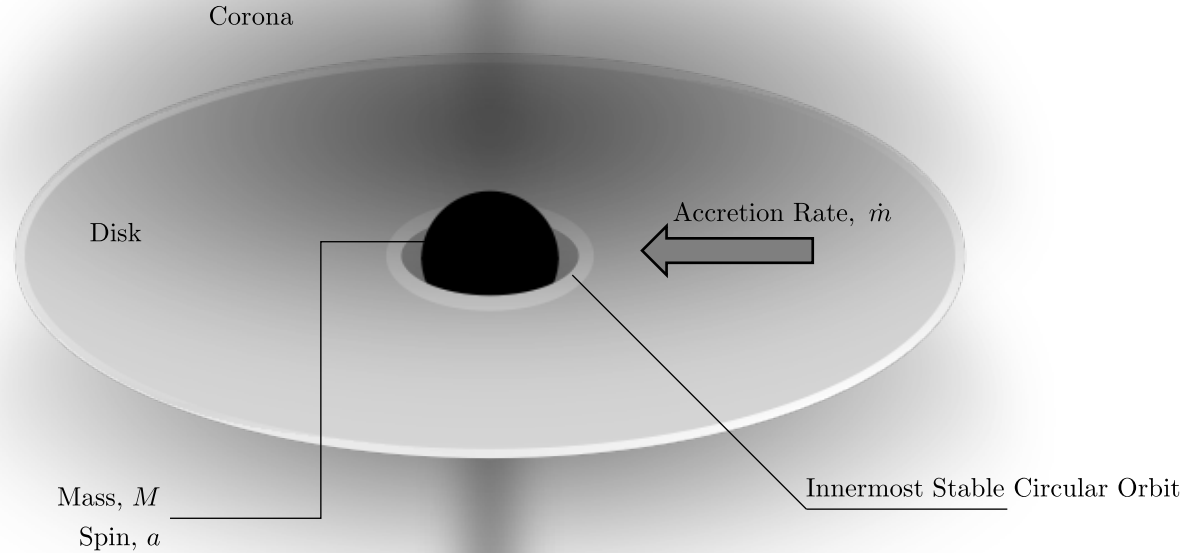
black hole basics



And in many systems, a relativistic *jet* launches perpendicular to the disk.

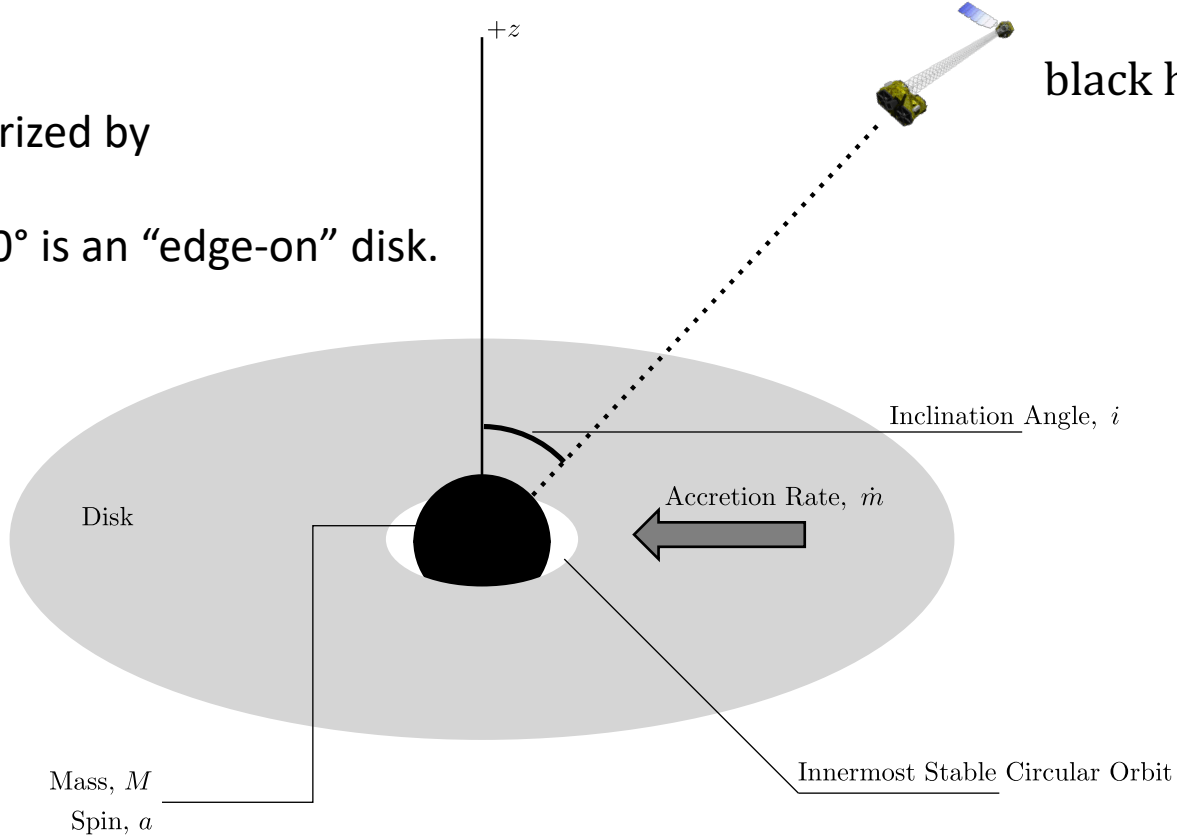
Jet

black hole basics



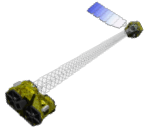
Observation is characterized by
the *inclination angle*:

0° is a “face-on” disk, 90° is an “edge-on” disk.

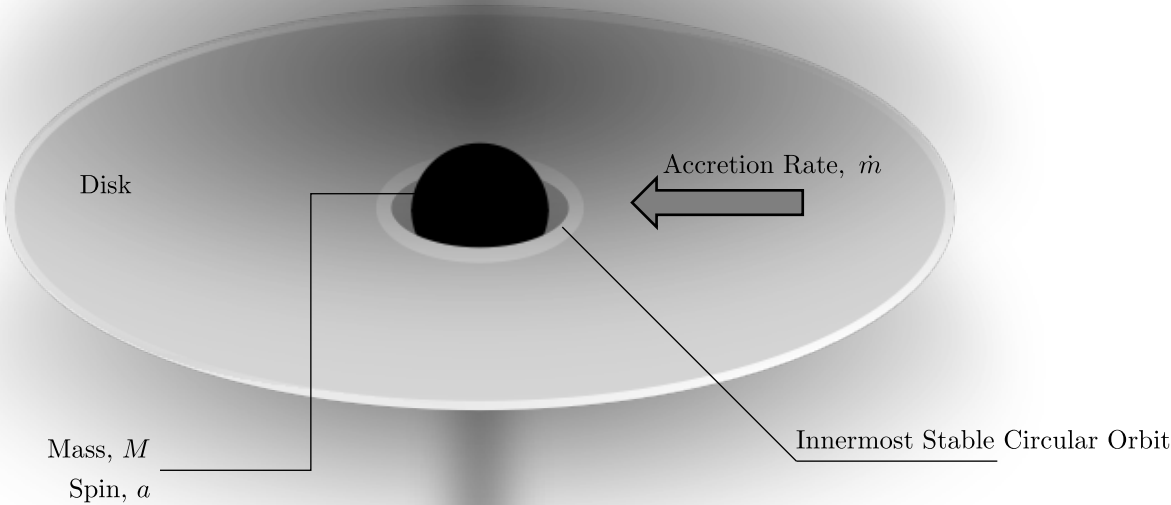


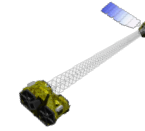
What does this X-ray telescope see?

Jet



black hole basics

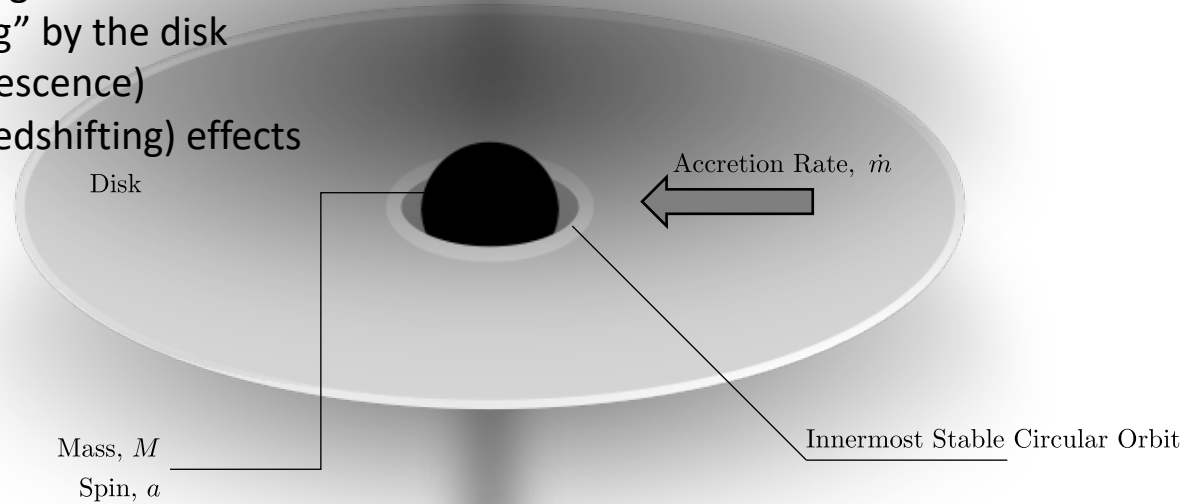


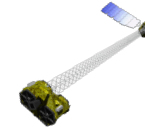


What does this X-ray telescope see?

The complex interactions between:

- thermal radiation from the disk
- Compton upscattering in the corona
- Compton downscattering in the disk
- reflection/“reprocessing” by the disk
- atomic processes (fluorescence)
- SR (boosting) and GR (redshifting) effects





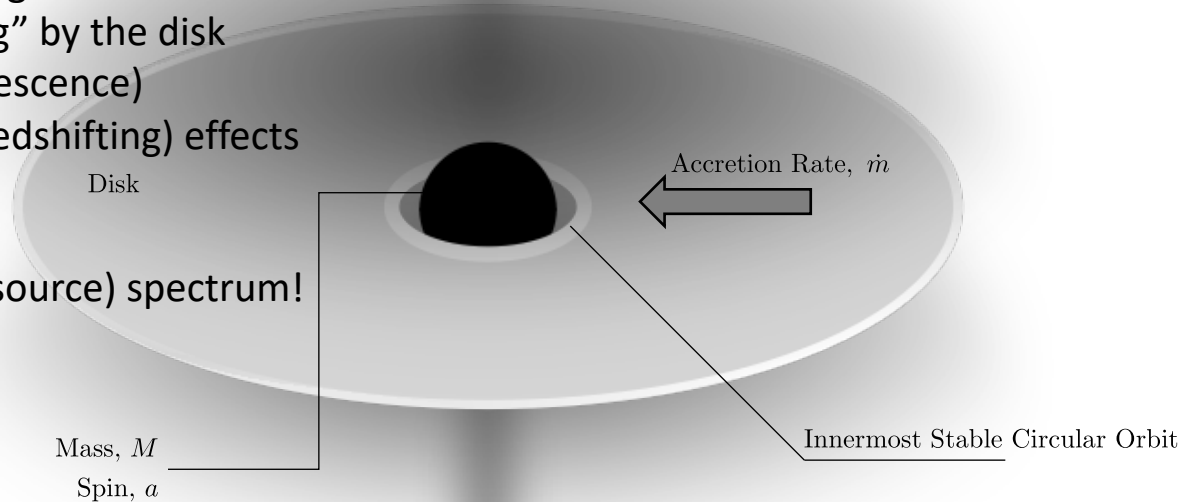
Jet

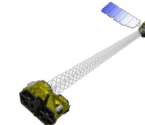
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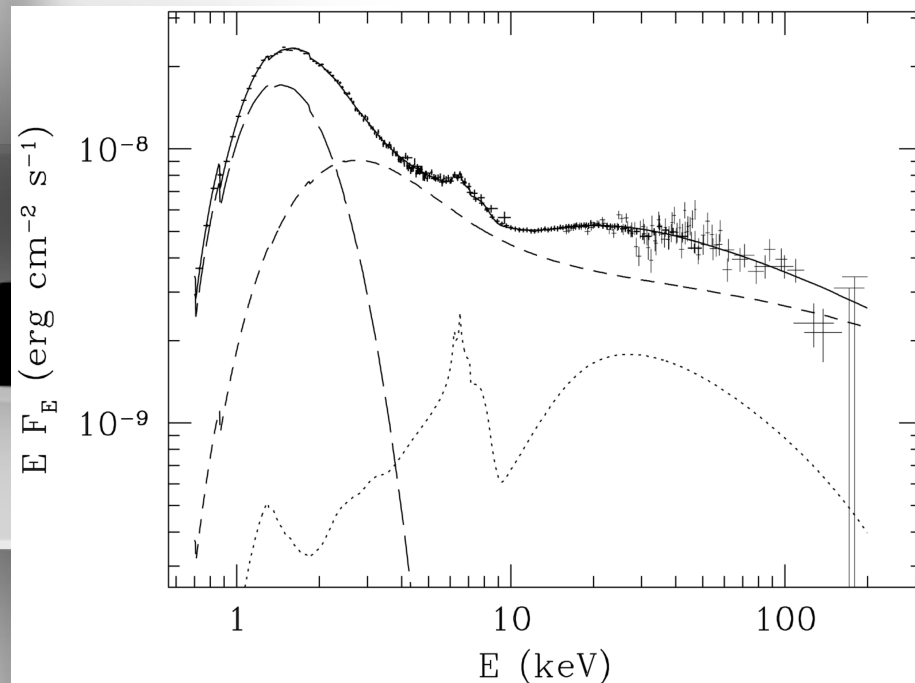
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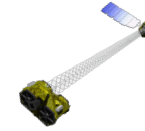
Disk

Mass, M
Spin, a



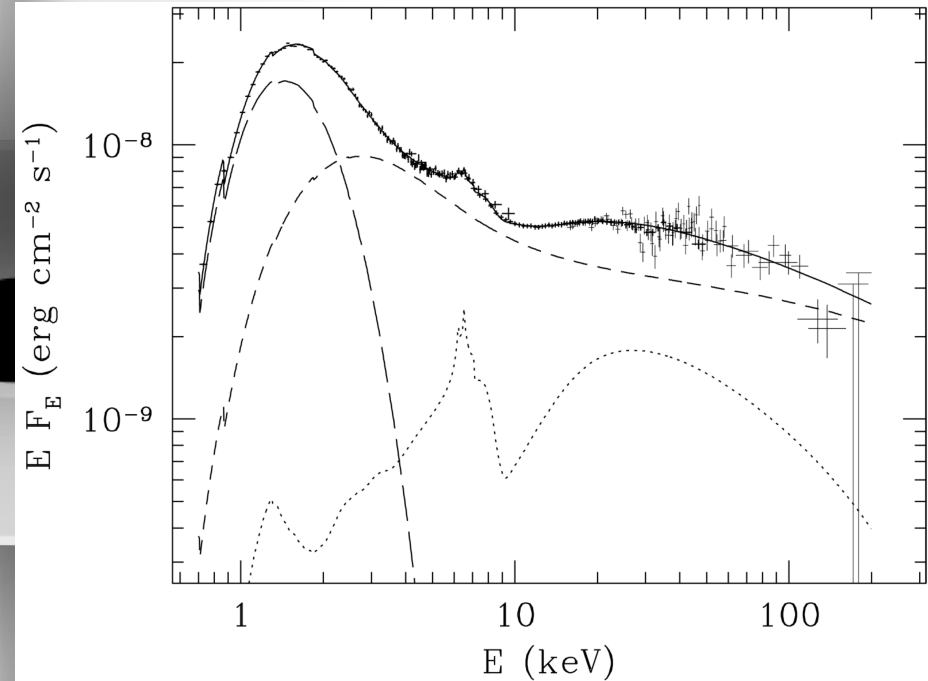
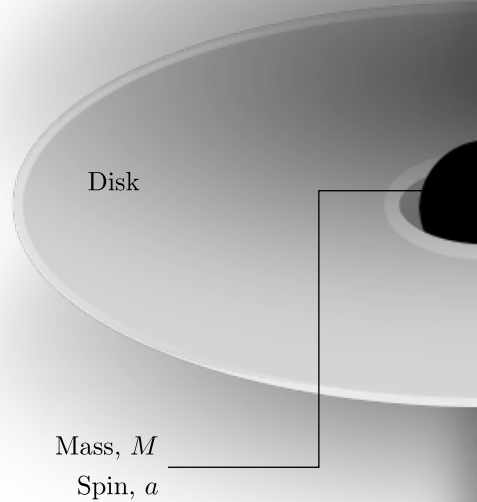
ASCA+RXTE spectra of Cyg X-1
(Gierliński & Zdziarski, 1999)





In order to model this spectrum...

We must first understand the nature of the accretion flow.



ASCA+RXTE spectra of Cyg X-1
(Gierliński & Zdziarski, 1999)

General Relativistic Magnetohydrodynamics (GRMHD)

$$\frac{1}{\sqrt{-g}} \partial_\mu (\sqrt{-g} \rho u^\mu) = 0 \quad \text{conservation of mass}$$

$$\partial_t (\sqrt{-g} T^t_\nu) = -\partial_i (\sqrt{-g} T^i_\nu) + \sqrt{-g} T^\kappa_\lambda \Gamma^\lambda_{\nu\kappa} \quad \text{conservation of energy-momentum (4 equations)}$$

$$T^{\mu\nu}_{\text{MHD}} = (\rho + u + p + b^2) u^\mu u^\nu + \left(p + \frac{b^2}{2} \right) g^{\mu\nu} - b^\mu b^\nu \quad \text{ideal MHD tensor (zero fluid rest frame E field)}$$

$$\partial_t (\sqrt{-g} B^i) = \partial_j [\sqrt{-g} (b^j u^i - b^i u^j)] \quad \text{ideal MHD induction equation (Faraday's law + Ohm's law)}$$

$$\frac{1}{\sqrt{-g}} \partial_i (\sqrt{-g} B^i) = 0 \quad \text{no magnetic monopoles constraint}$$

$$p = (\Gamma - 1)u \quad \text{ideal gas equation of state (for closure)}$$

adiabatic index



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The HARM method:

A conservative, shock-capturing scheme which maintains a divergence-free magnetic field (Gammie, McKinney, & Tóth, 2003).



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The HARM method:

1. Define a vector of conserved variables:

$$\mathbf{U} \equiv \sqrt{-g} (\rho u^t, T^t_t, T^t_i, B^i)$$

2. Define a vector of “primitive” variables:

$$\mathbf{P} \equiv (\rho, u, v^i, B^i)$$

3. Re-cast equations into flux-conservative form:

$$\partial_t \mathbf{U}(\mathbf{P}) = -\partial_i \mathbf{F}^i(\mathbf{P}) + \mathbf{S}(\mathbf{P})$$

4. Update conserved variables (explicitly integrate above equation over one time step)

5. Recover primitives from conserved variables via multidimensional Newton-Raphson.

$$\mathbf{P}_{t+\Delta t} = g(\mathbf{U}_{t+\Delta t})$$



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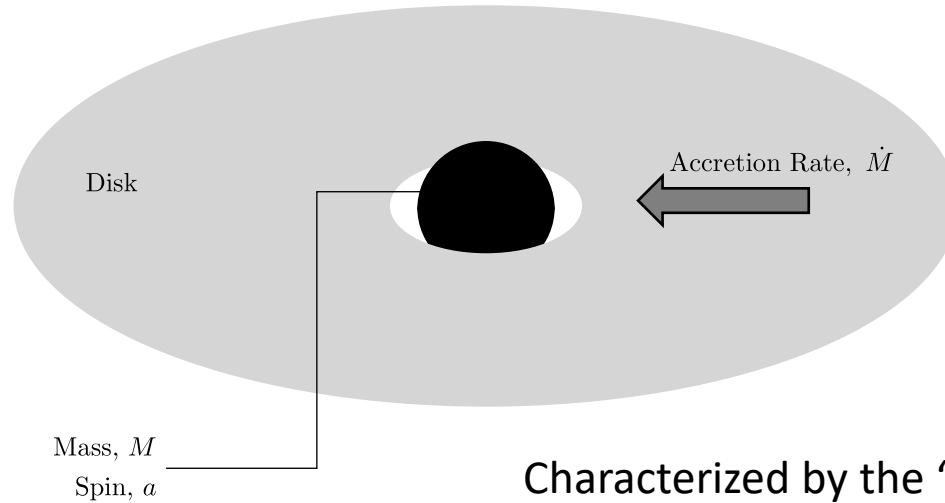
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To model moderately-accreting systems of interest (XRBs or AGN), we require GRRMHD (+ radiation)... or some means by which to mimic radiative losses.



General Relativistic Magnetohydrodynamics (GRMHD)

HARM3D (Noble, Krolik & Hawley 2009):

A 3D extension to the (original, 2D) HARM code,
including an energy *sink* term in the stress-energy conservation equations.



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Gas is cooled over an orbital time scale to achieve a target temperature, itself chosen to achieve a target *aspect ratio* – that of a geometrically thin disk.

$$T_{\text{target}} = \frac{\pi}{2} \frac{R_z(r)}{r} \left[\frac{H(r)}{r} \right]^2$$

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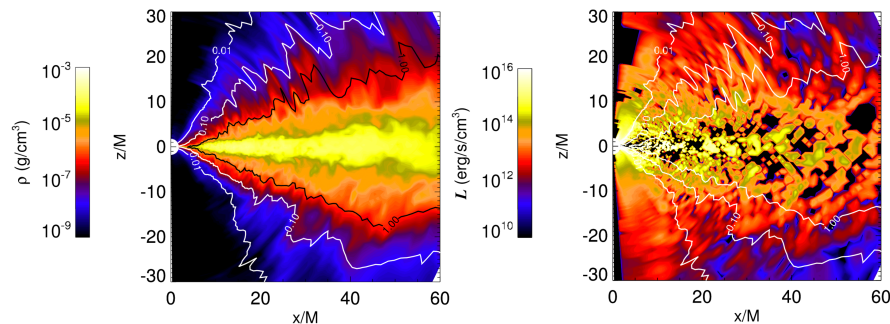
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“ThinHR” simulation series:

Achieves a thin disk in inflow equilibrium.
Naturally produces an extended corona.
Resolves the magneto-rotational instability.



Two microphysical improvements to HARM3D:

(Kinch, Noble, Schnittman, & Krolik 2020)

Inverse Compton Coronal Cooling Function

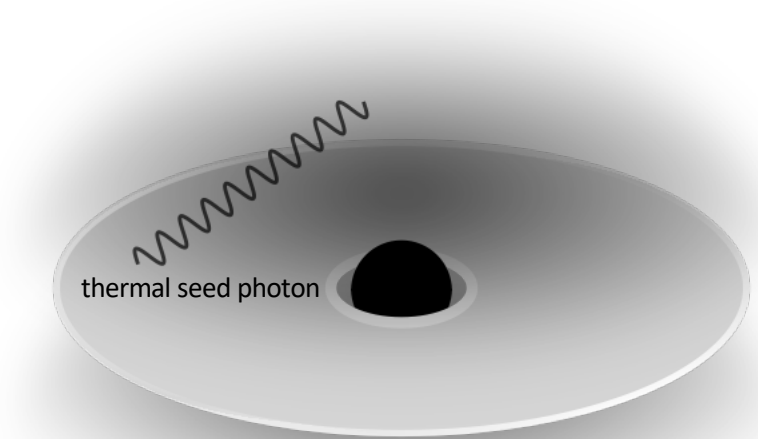


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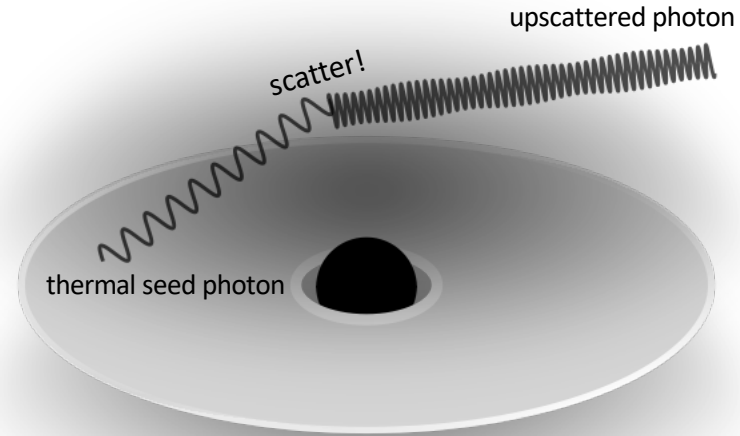


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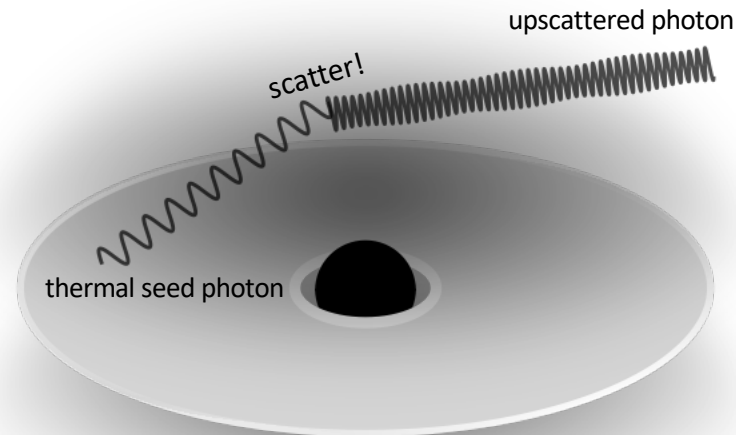
Two microphysical improvements to HARM3D:

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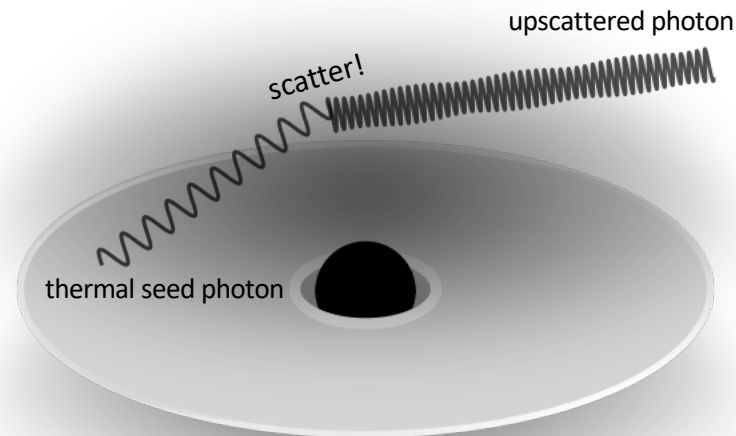
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The challenge: arrive at a reasonable approximation for the **radiation energy density**... without resorting to full transport.



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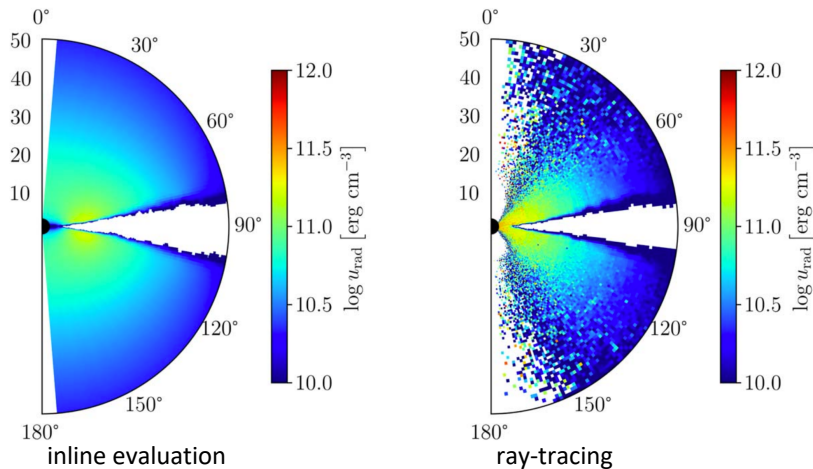
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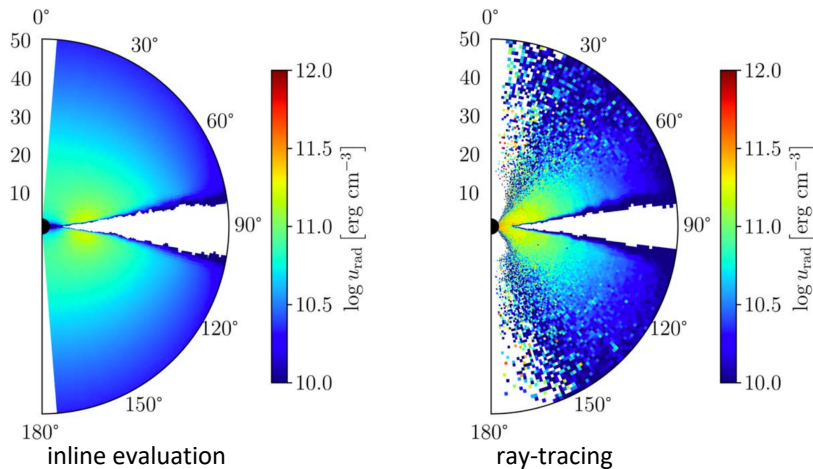
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Crucially important for modeling real black hole systems on human time scales.



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Two-Temperature Coronal Model

Turbulent energy eventually heats up the plasma *thermally* – how this heat is split between ions and electrons is a *difficult* plasma kinetics problem.



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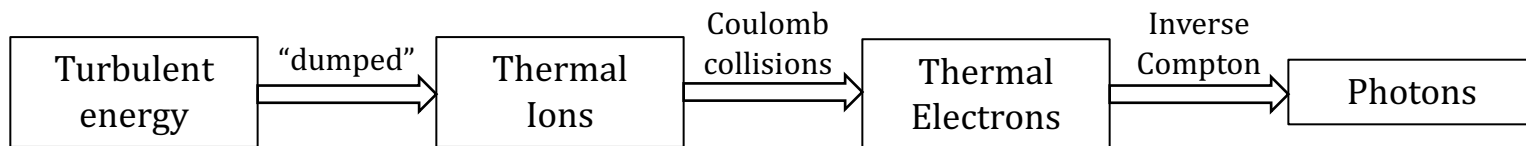
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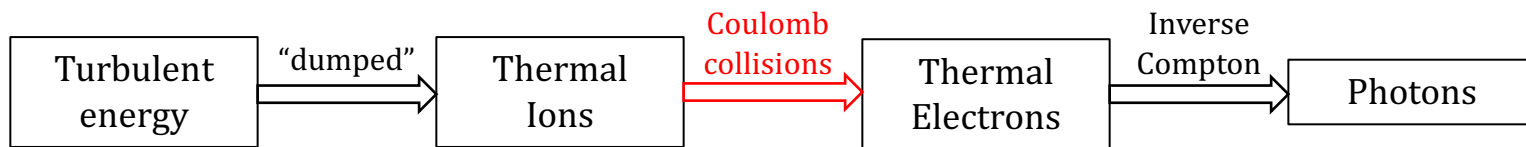
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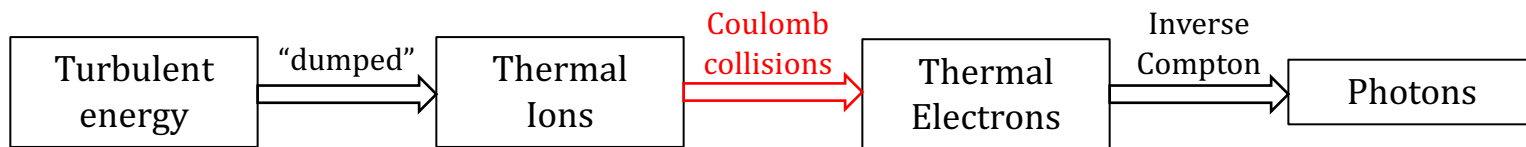
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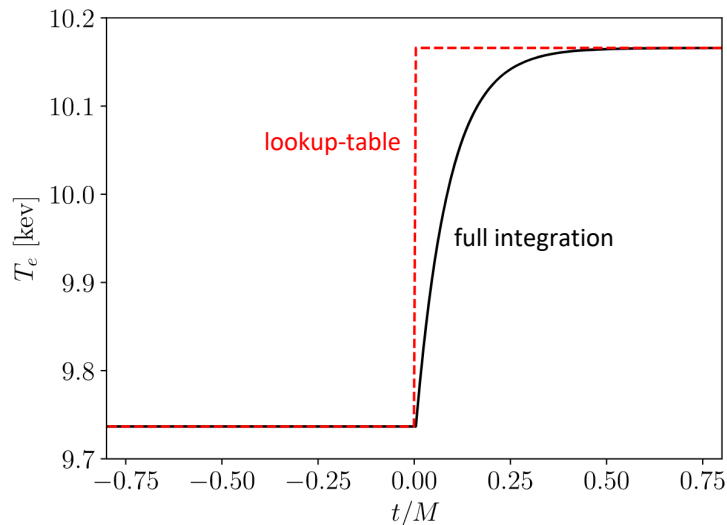
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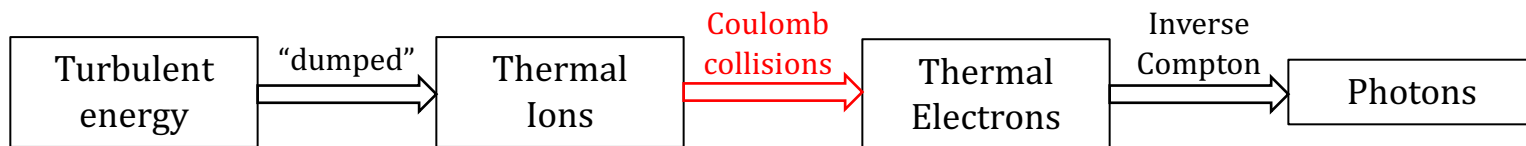
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- Thus we can simulate realistic black hole accretion flows.
- The next step is to generate synthetic X-ray spectra from these simulations.



X-Ray Postprocessing – Overview

- Relatively cool, dense disk treated with deterministic, plane-parallel radiation transport code PTRANSX:
 - Feautrier method
 - coupled to photoionization code XSTAR
 - fully relativistic Compton using compy

corona



disk



X-Ray Postprocessing – Overview

corona

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X-Ray Postprocessing – Overview

corona

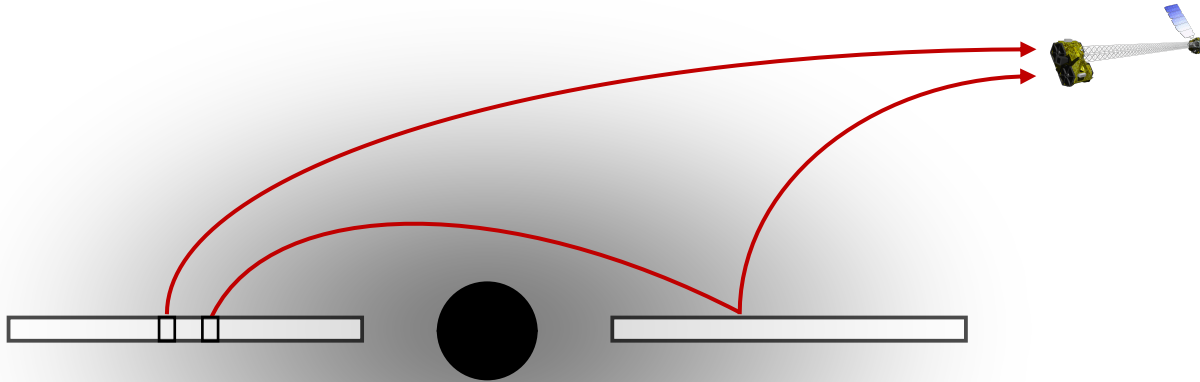
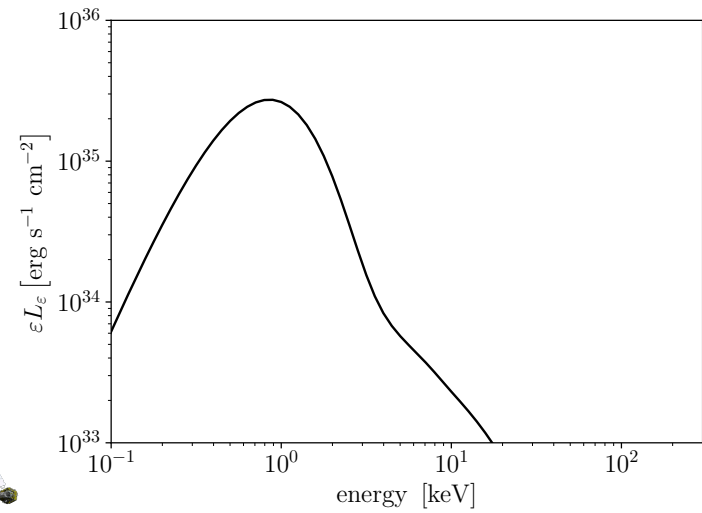
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- Two codes handling two different regimes, interfaced to each other at disk/corona boundary.



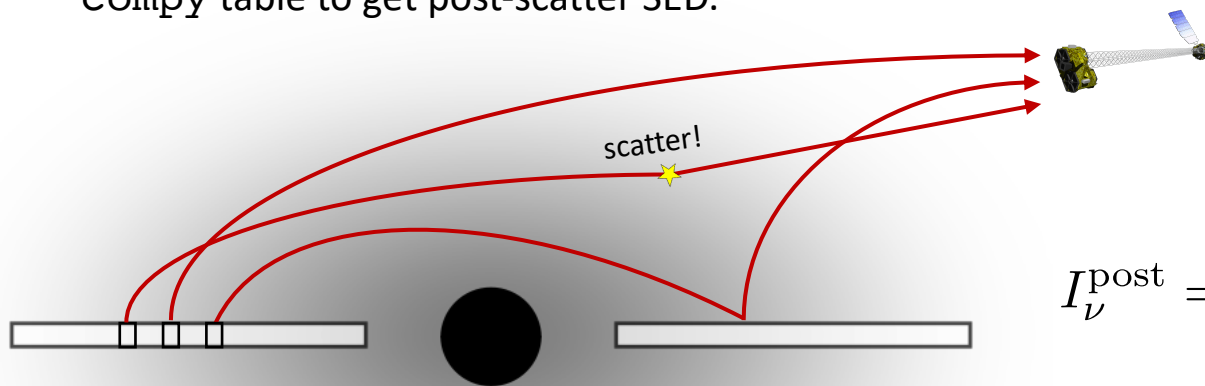
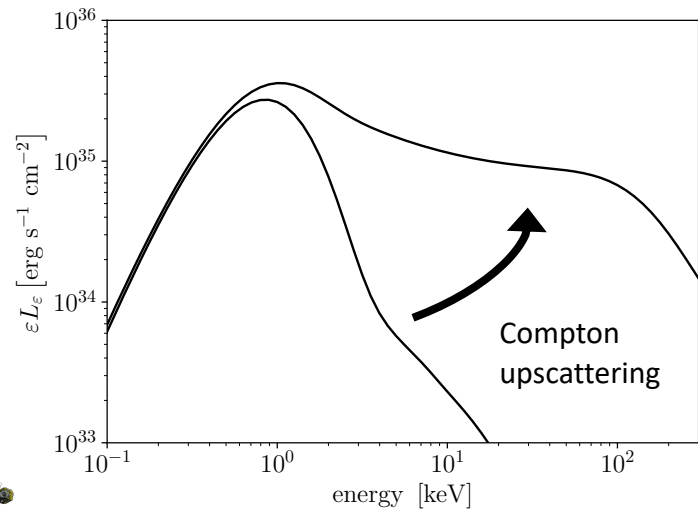
X-Ray Postprocessing – Corona

1. Assume each plane-parallel slab of disk radiates a blackbody according to its vertically-integrated cooling rate.
2. Use *Pandurata* to transport photon packets to distant observers (emitter-to-observer ray-tracing).



X-Ray Postprocessing – Corona

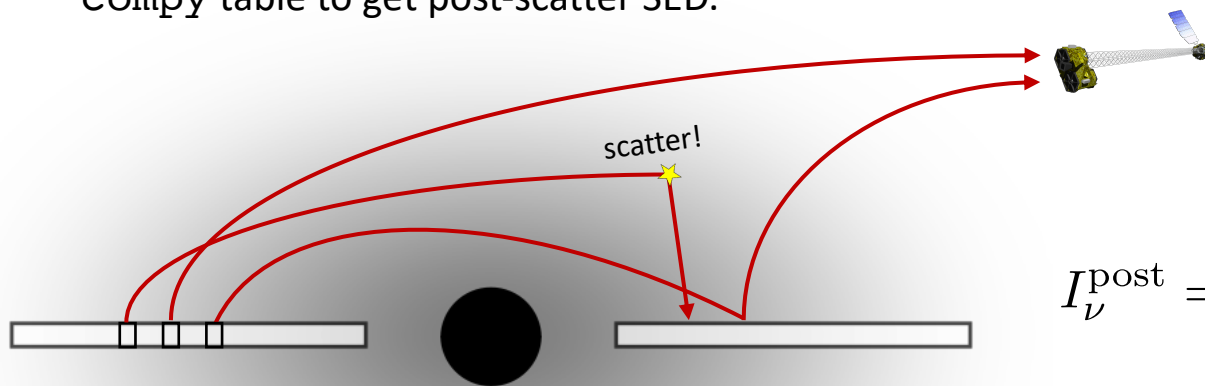
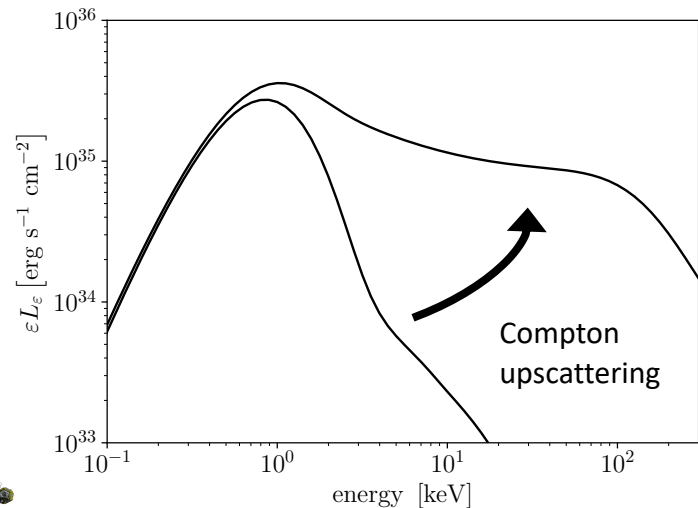
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X-Ray Postprocessing – Corona

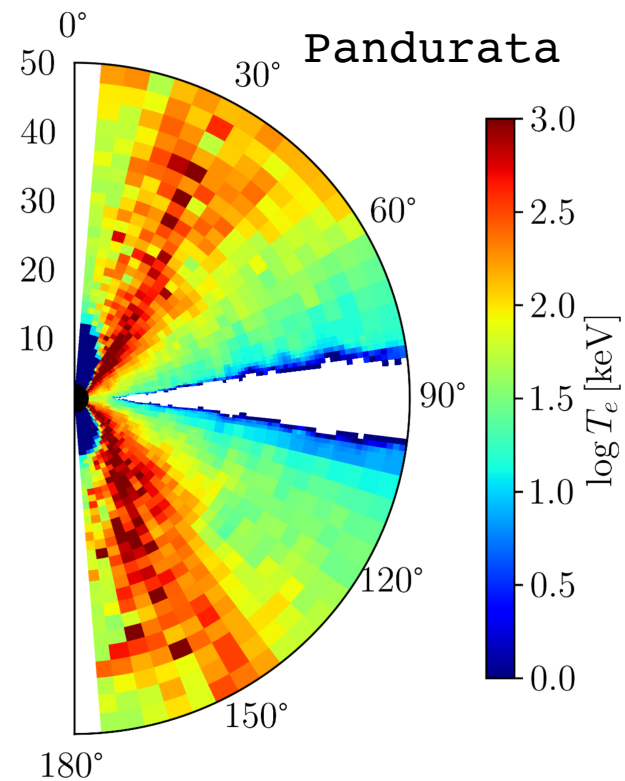
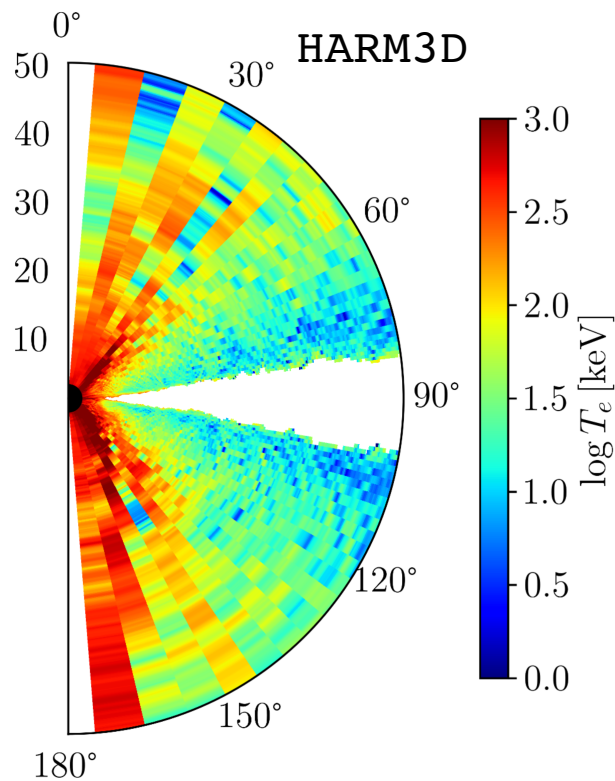
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X-Ray Postprocessing – Corona

4. Use Newton-Raphson iterations in every coronal *sector* to match HARM3D's cooling rate with Pandurata's electron temperature.

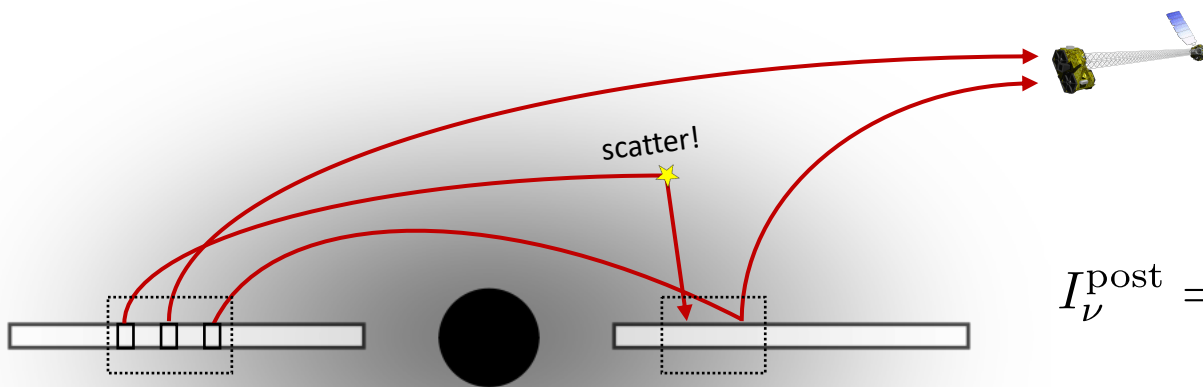
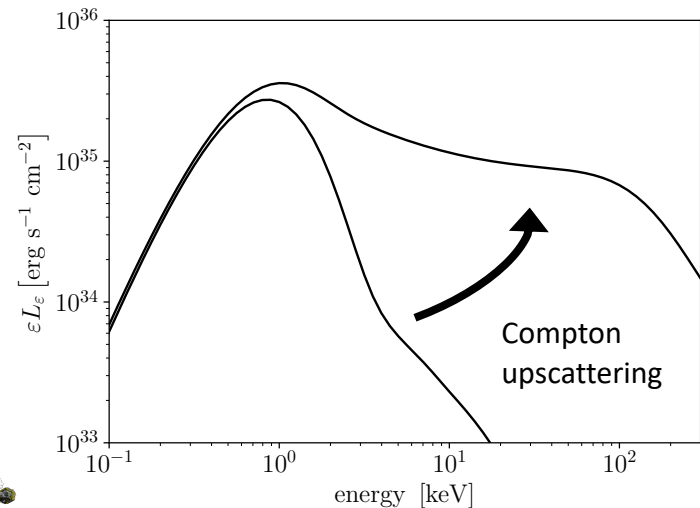


X-Ray Postprocessing – Corona + Disk

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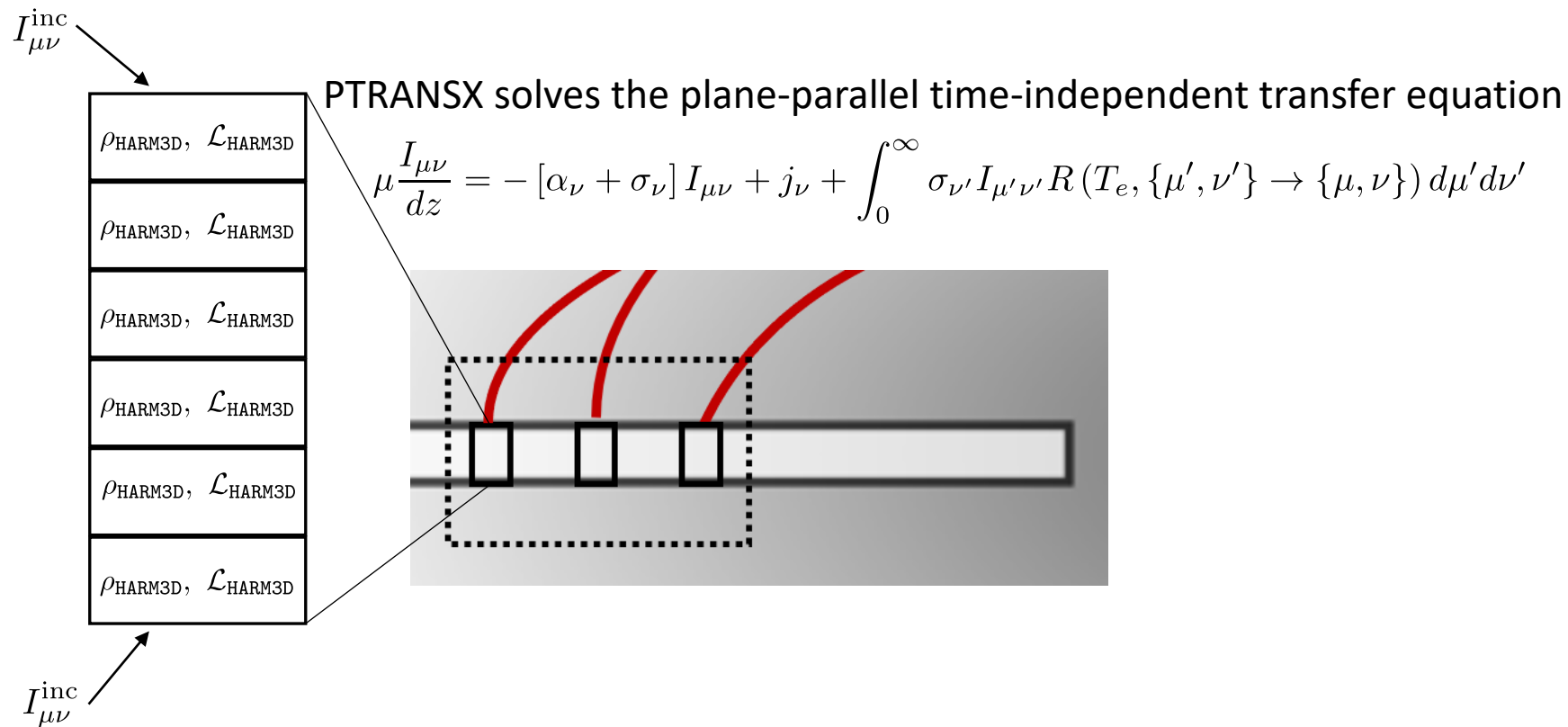
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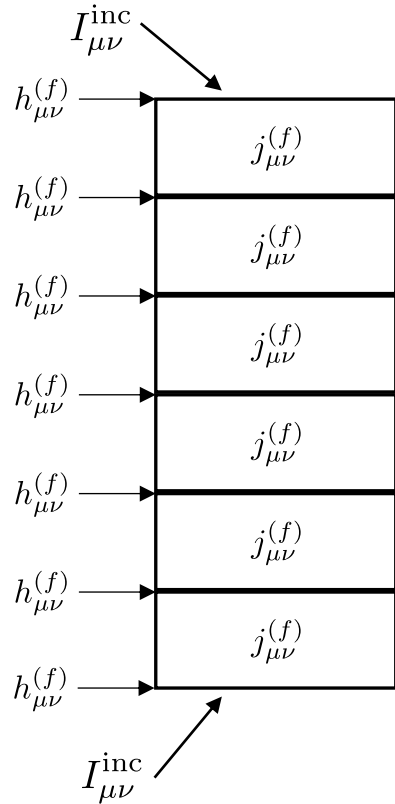


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X-Ray Postprocessing – Disk



X-Ray Postprocessing – Disk



PTRANSX solves the plane-parallel time-independent transfer equation

$$\mu \frac{I_{\mu\nu}}{dz} = -[\alpha_\nu + \sigma_\nu] I_{\mu\nu} + j_\nu + \int_0^\infty \sigma_{\nu'} I_{\mu'\nu'} R(T_e, \{\mu', \nu'\} \rightarrow \{\mu, \nu\}) d\mu' d\nu'$$

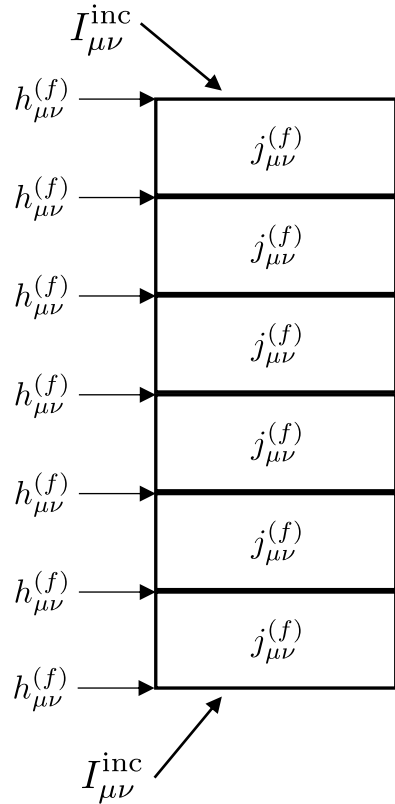
via the Feautrier method – splitting the radiation field into symmetric and anti-symmetric averages:

$$\begin{aligned} j_{\mu\nu}^{(f)} &= \frac{1}{2} (I_{\mu\nu}^+ + I_{\mu\nu}^-) \\ h_{\mu\nu}^{(f)} &= \frac{1}{2} (I_{\mu\nu}^+ - I_{\mu\nu}^-) \end{aligned} \quad 0 \leq \mu \leq 1$$

Subject to *incident specific intensity* boundary conditions set by Pandurata.



X-Ray Postprocessing – Disk



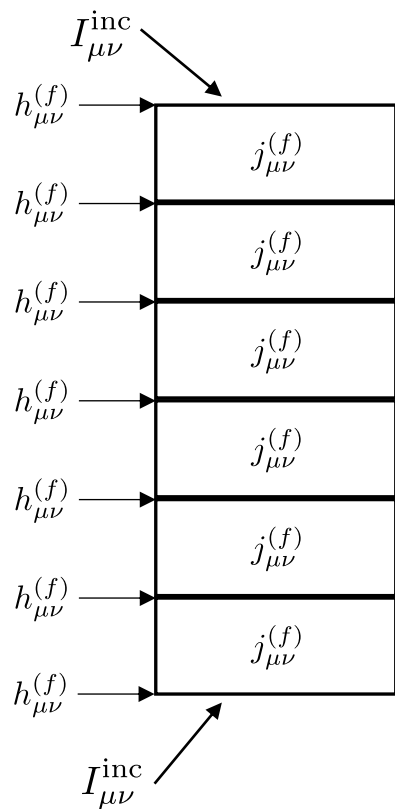
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X-Ray Postprocessing – Disk



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absorption opacity includes:

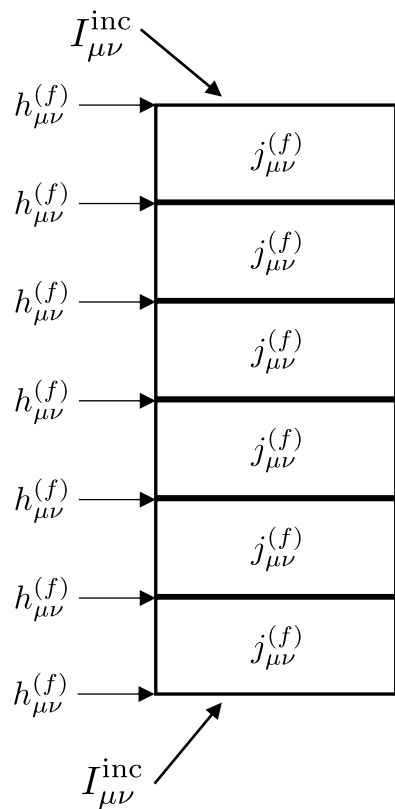
free-free, bound-free photoionization edges

emissivity includes:

free-free, recombination continuum, line emission



X-Ray Postprocessing – Disk



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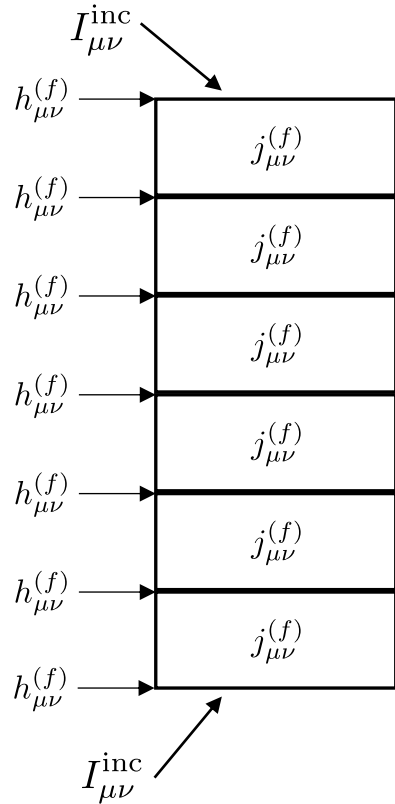
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We use the photoionization code XSTAR to determine the *photoionization equilibrium ionization balance* and corresponding absorption opacity and emissivity...

for a given temperature and radiation field (and density).



X-Ray Postprocessing – Disk



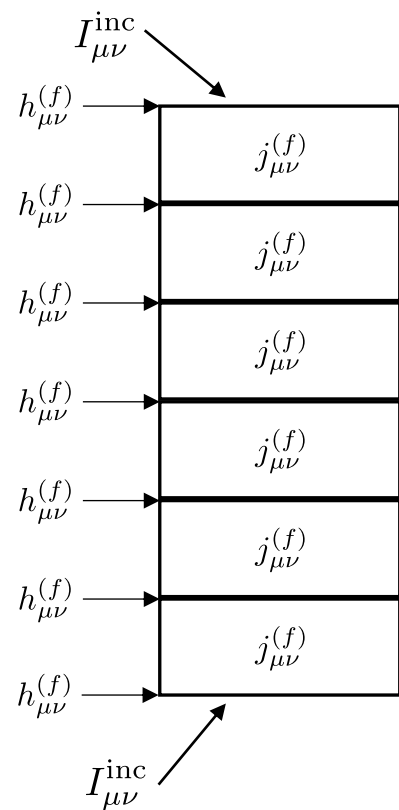
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X-Ray Postprocessing – Disk



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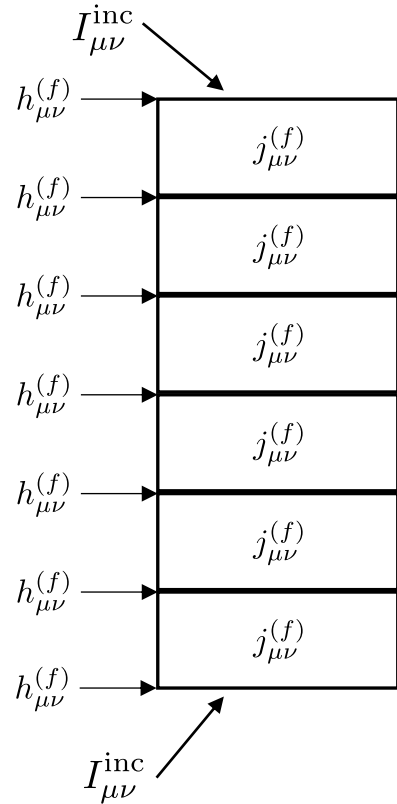
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X-Ray Postprocessing – Disk



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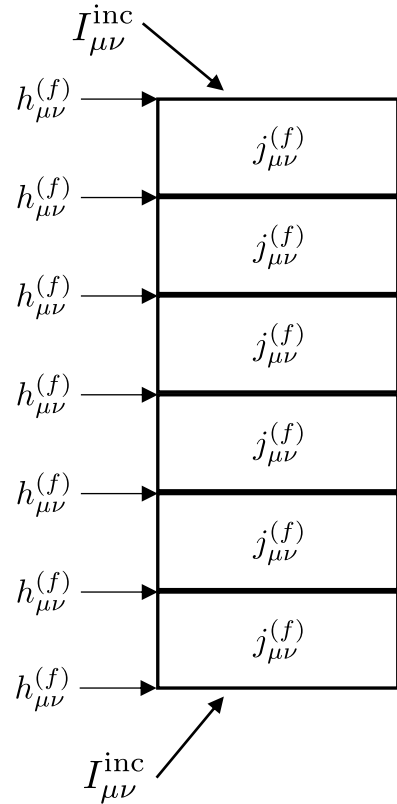
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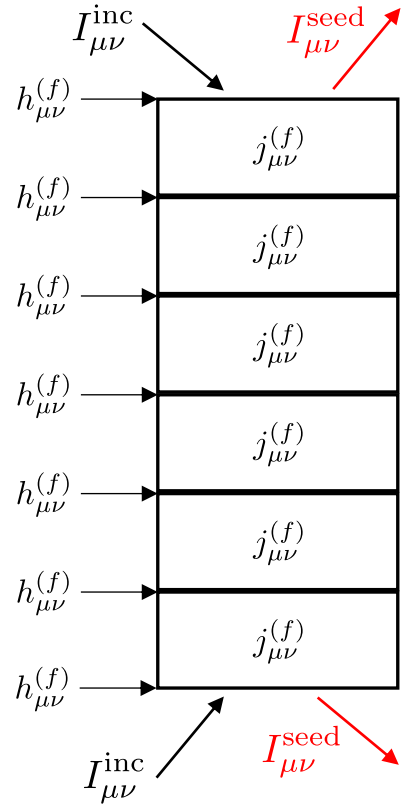
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5. Compute the *energy-conserving, photoionization equilibrium-consistent* outgoing seed photon spectrum.

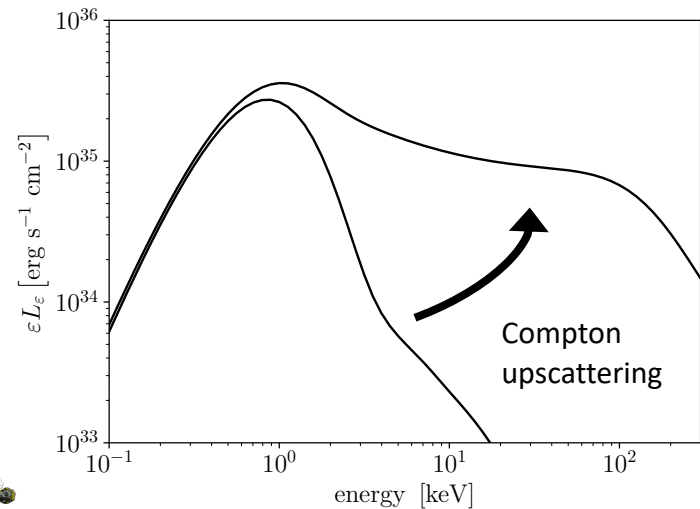
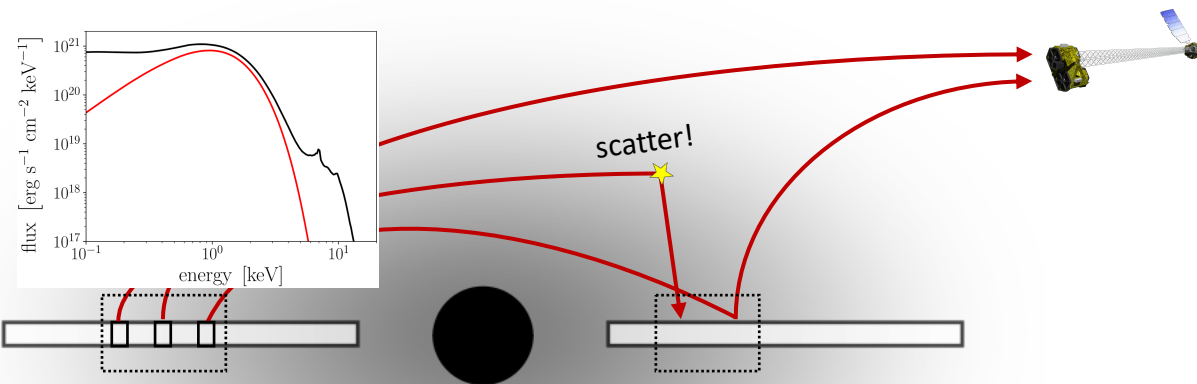


X-Ray Postprocessing – Corona + Disk

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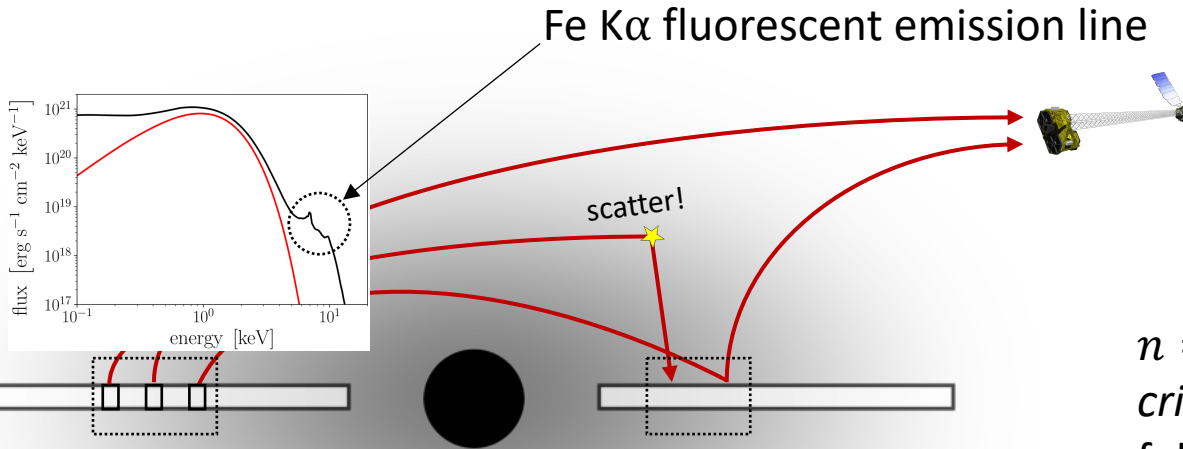
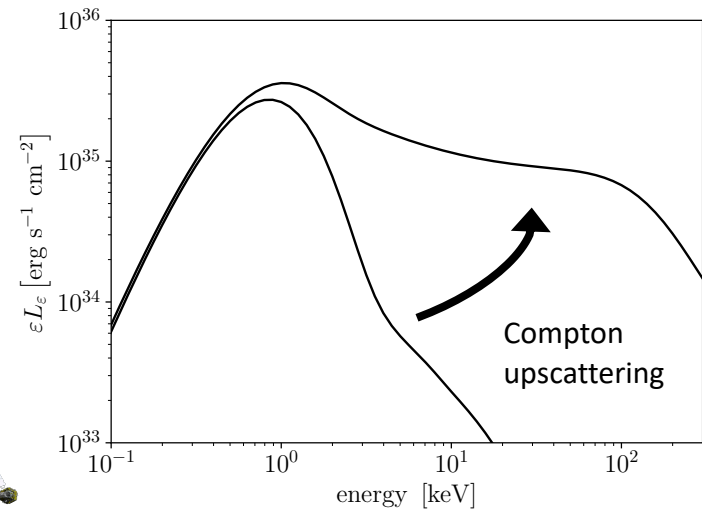


X-Ray Postprocessing – Corona + Disk

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$n = 2 \rightarrow n = 1$ Fe transition:
critically important X-ray diagnostic,
follows from photo-ejection of
K shell ($n = 1$) electron.



X-Ray Postprocessing – Disk

$I_{\mu\nu}^{\text{inc}}$

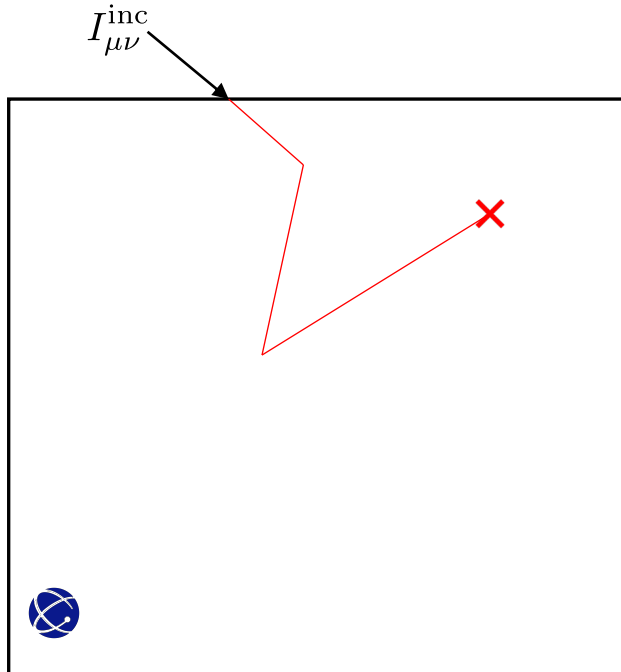


Auxiliary Monte Carlo code response –

1. Use PTRANSX output opacity and temperature structure for each plane-parallel slab.



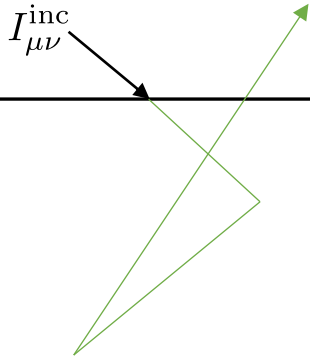
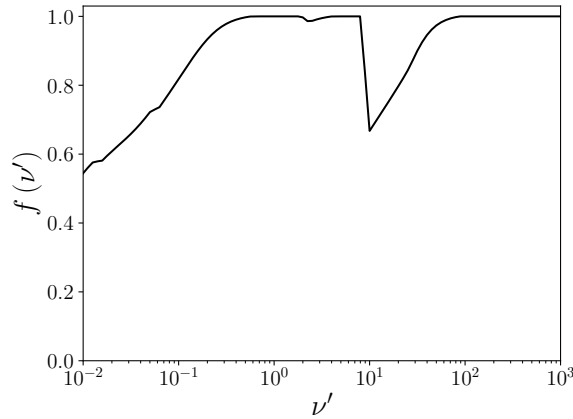
X-Ray Postprocessing – Disk



Auxiliary Monte Carlo code response –

1. Use PTRANSX output opacity and temperature structure for each plane-parallel slab.
2. Shoot photons in at each frequency grid-point and record the fraction that make it out (either side), i.e., the *albedo*.

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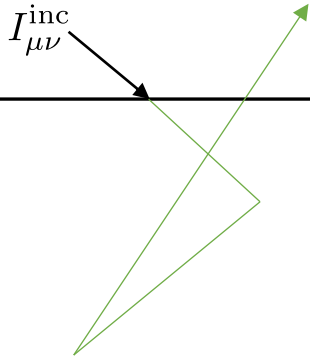
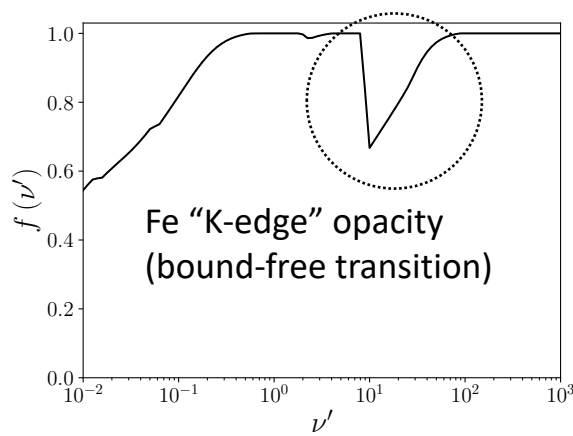


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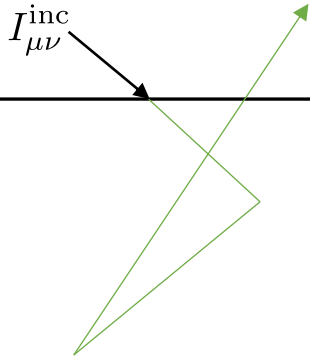
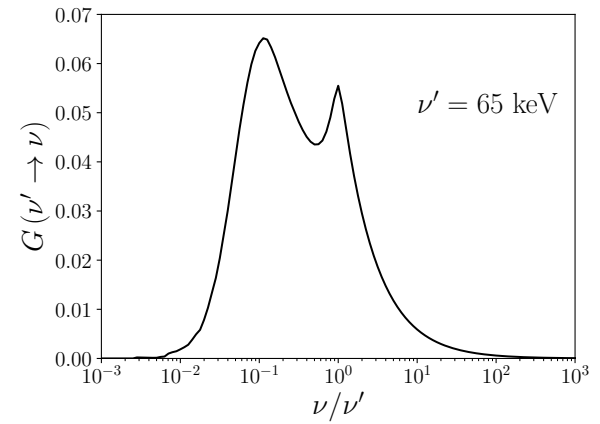
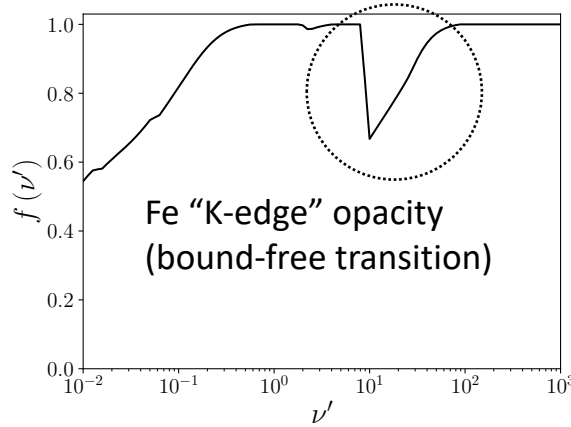


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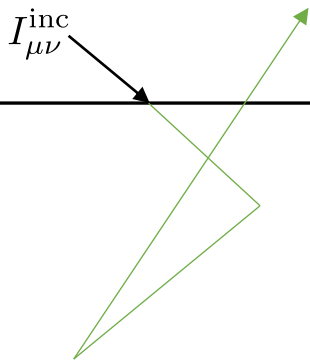
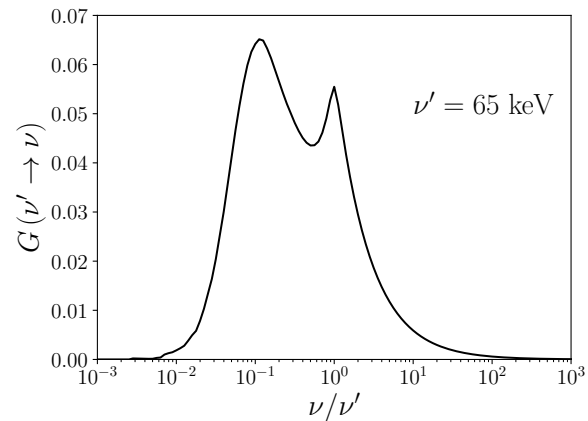
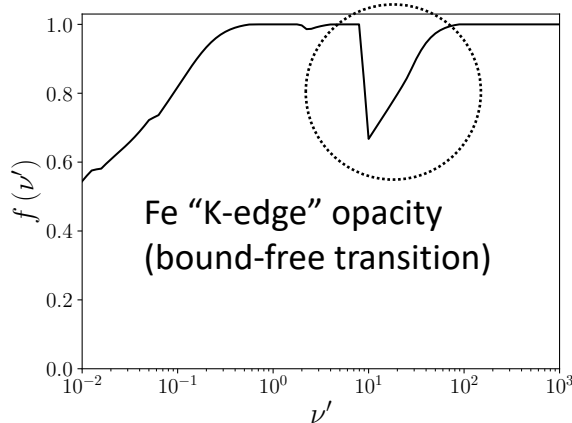


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3. Also record the distribution of outgoing frequencies for each incoming frequency (including transmission).



X-Ray Postprocessing – Disk



Auxiliary Monte Carlo code response –

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2. Shoot photons in at each frequency grid-point and record the fraction that make it out (either side), i.e., the *albedo*.
3. Also record the distribution of outgoing frequencies for each incoming frequency (including transmission).
4. When a photon packet strikes the disk during Pandurata ray-tracing, *reduce* level by albedo and convolve with interpolated distribution:

$$I_{\nu}^{\text{out}} = \int_0^{\infty} I_{\nu'}^{\text{inc}} f(\nu') G(\nu' \rightarrow \nu) d\nu'$$

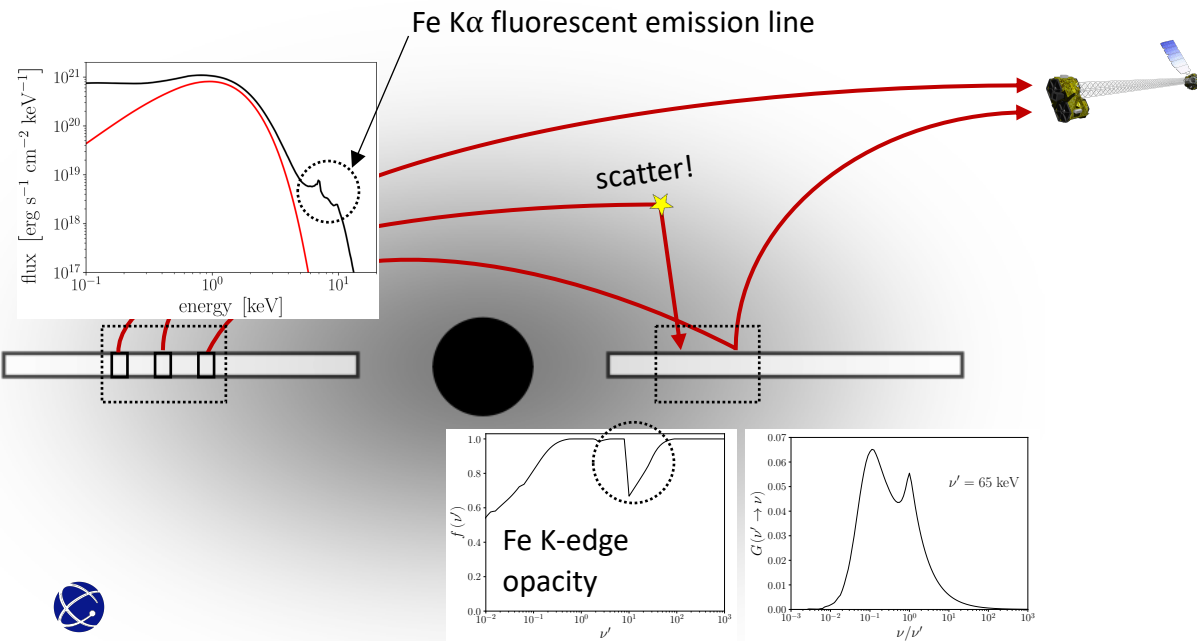
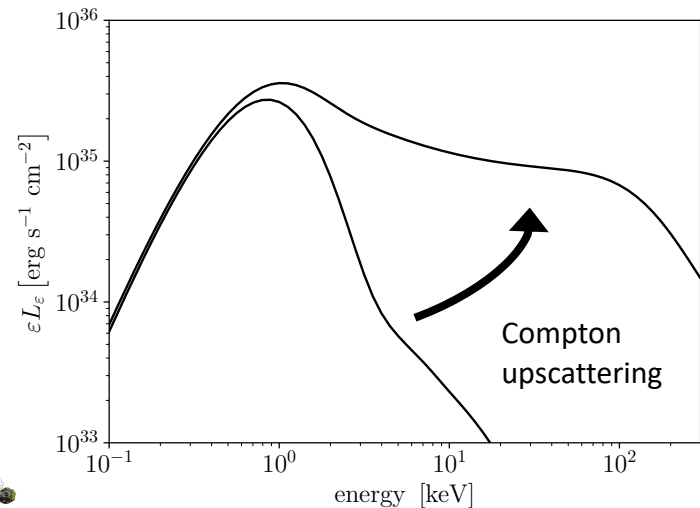


X-Ray Postprocessing – Corona + Disk

We still need a self-consistent treatment for:

The seed photon spectrum (not simply a blackbody).

How to transform a photon packet striking the disk surface.

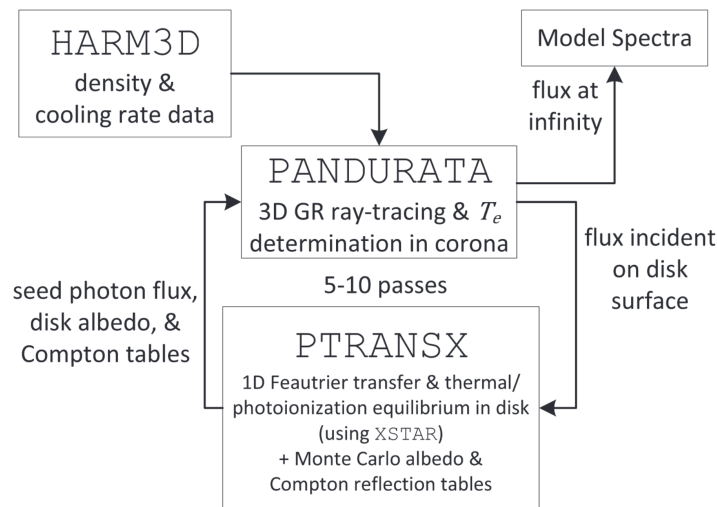
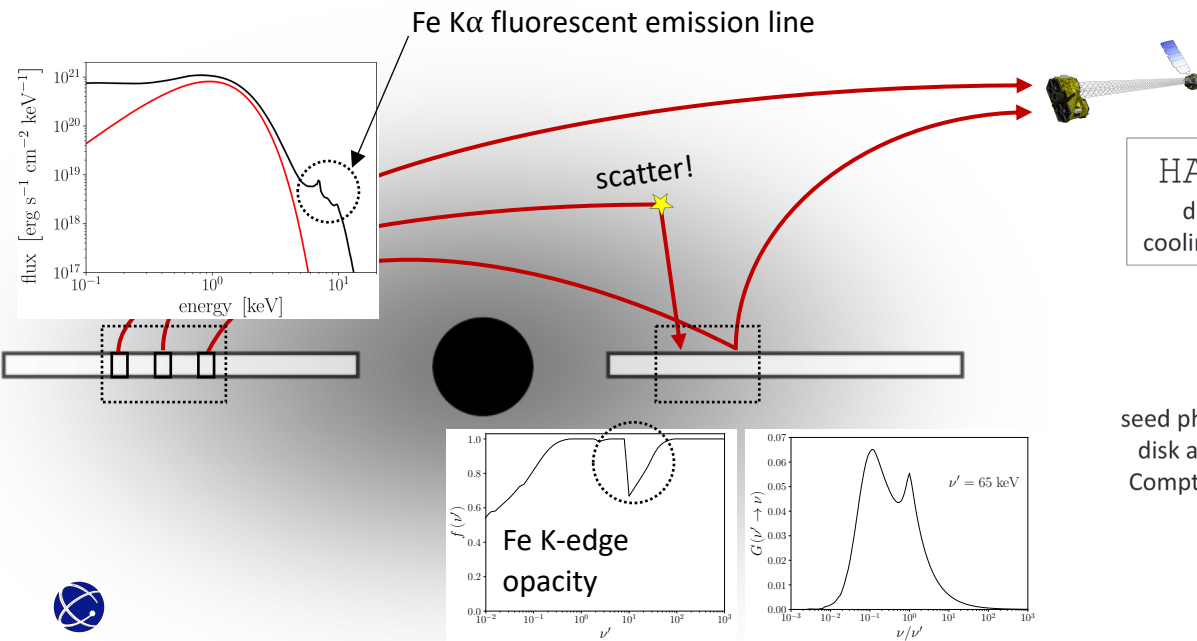
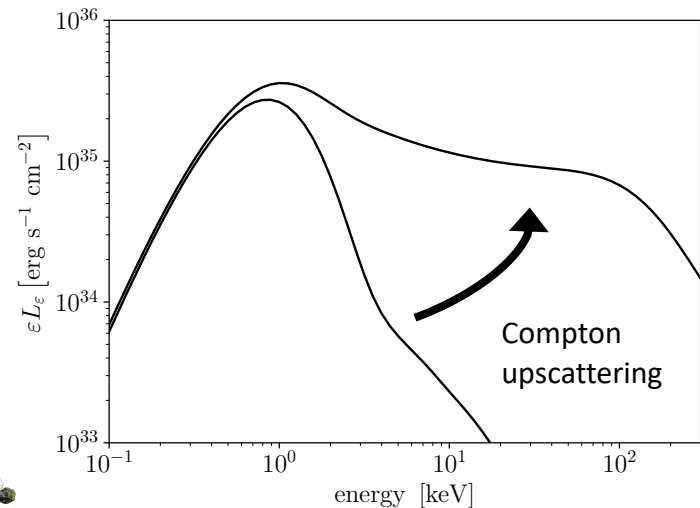


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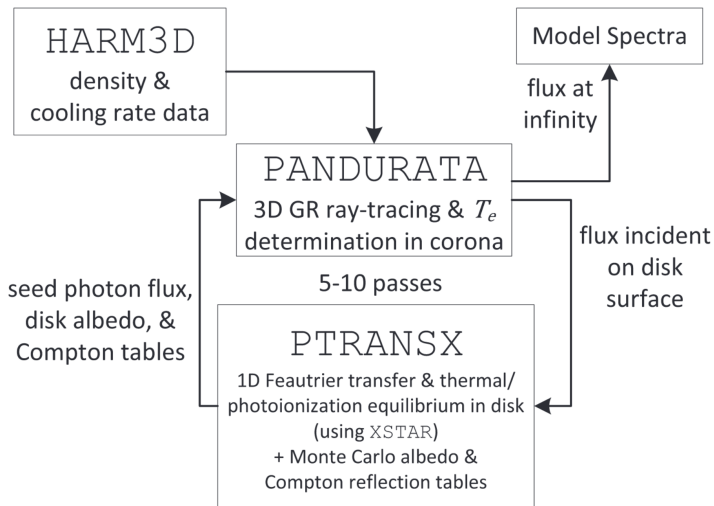
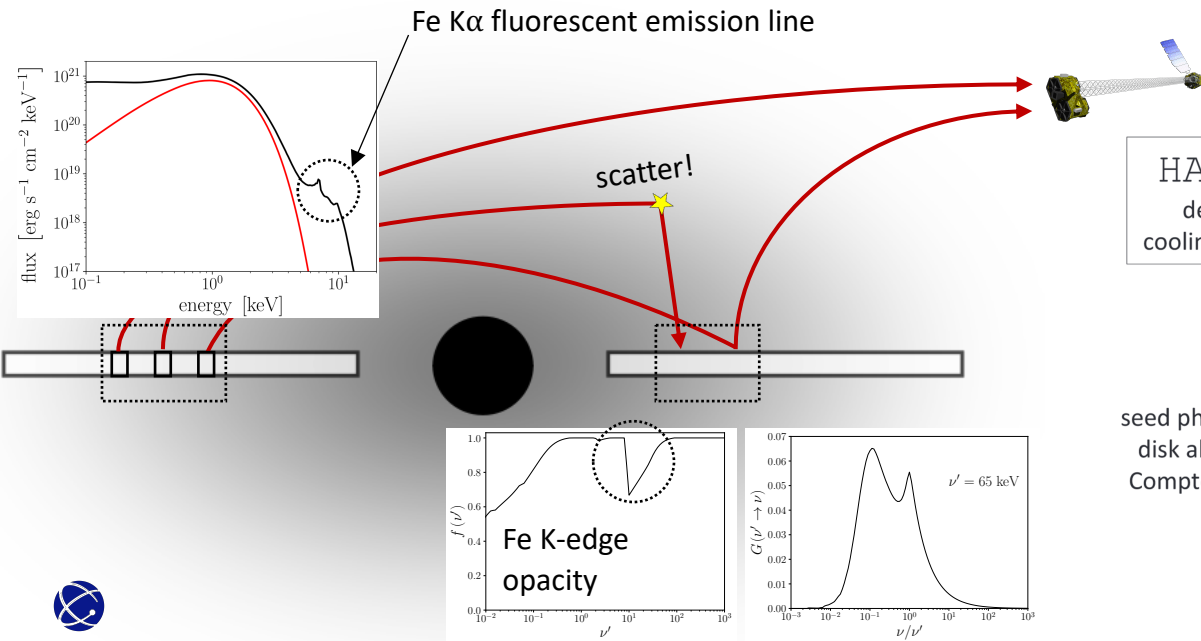
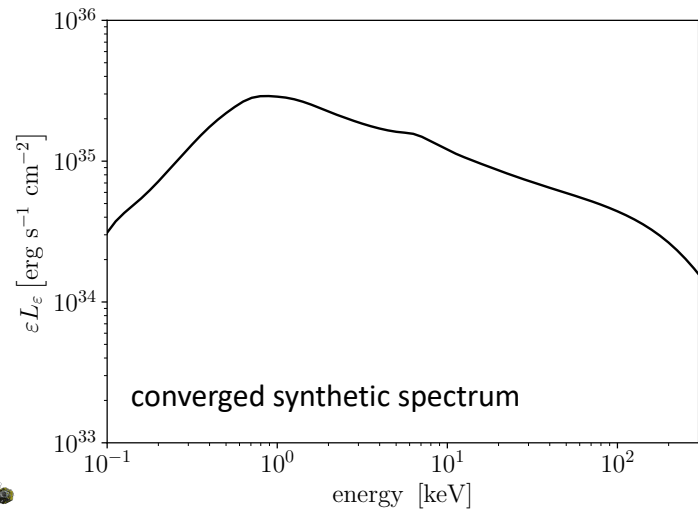


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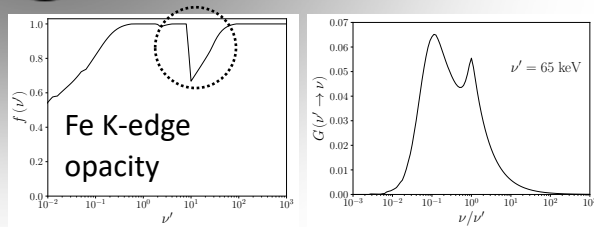
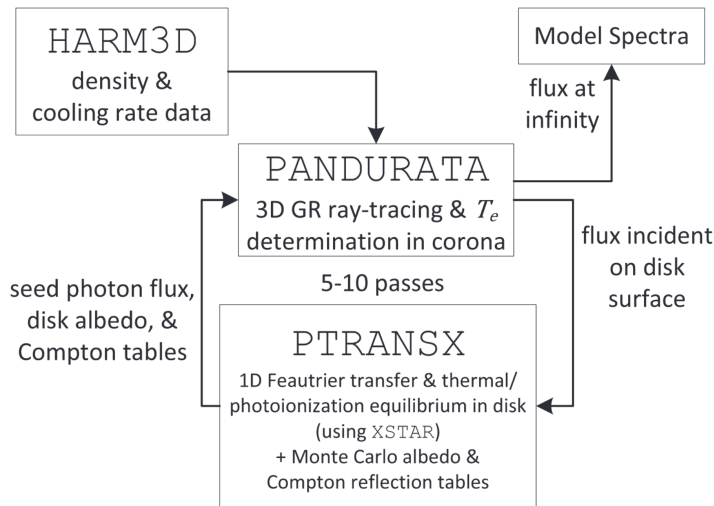
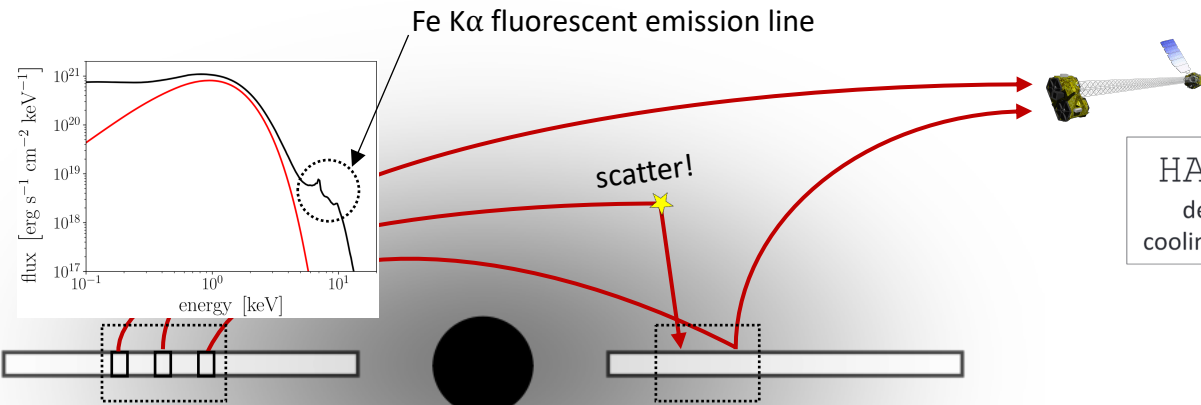
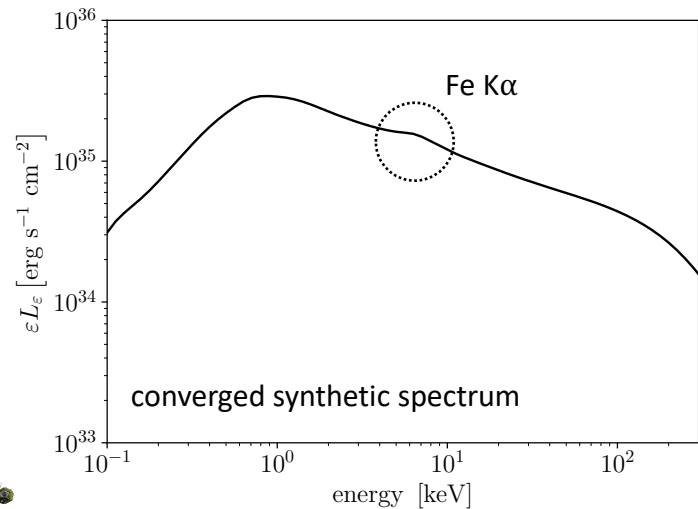


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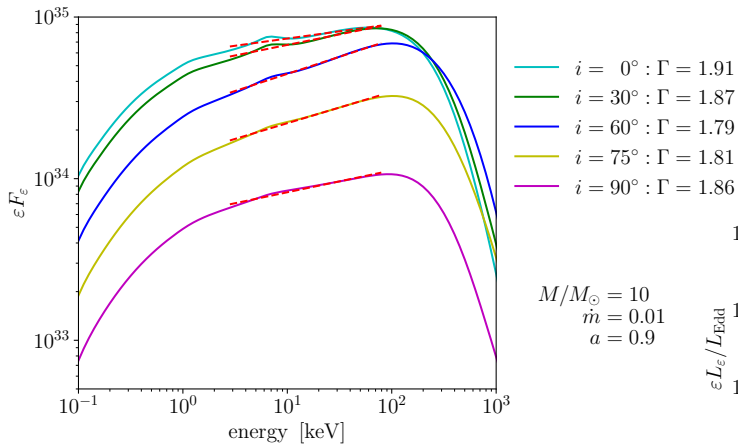
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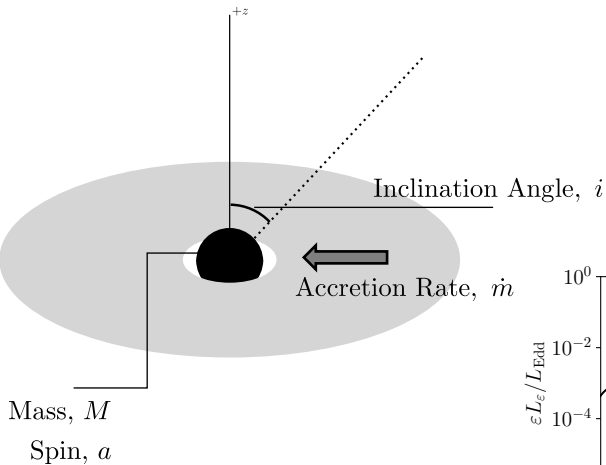
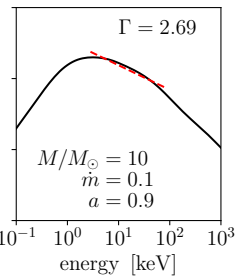
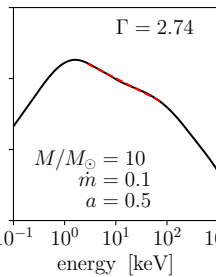
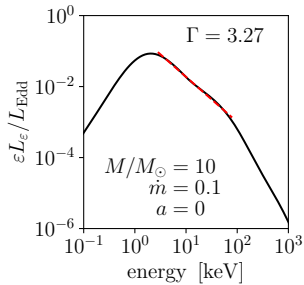
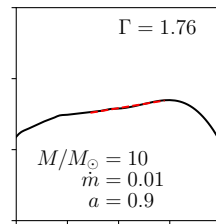
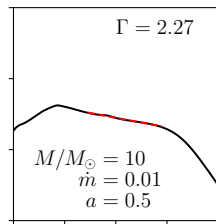
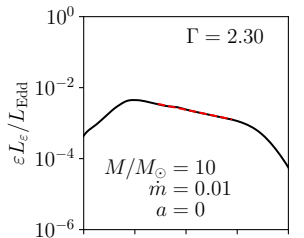
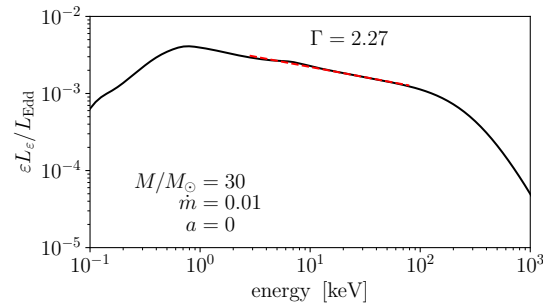
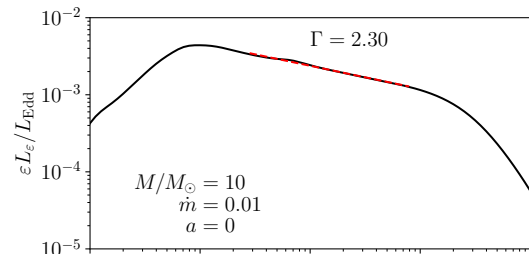
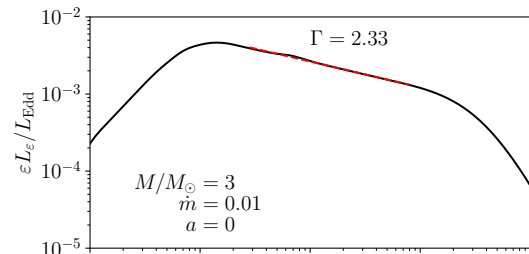
How to transform a photon packet striking the disk surface.



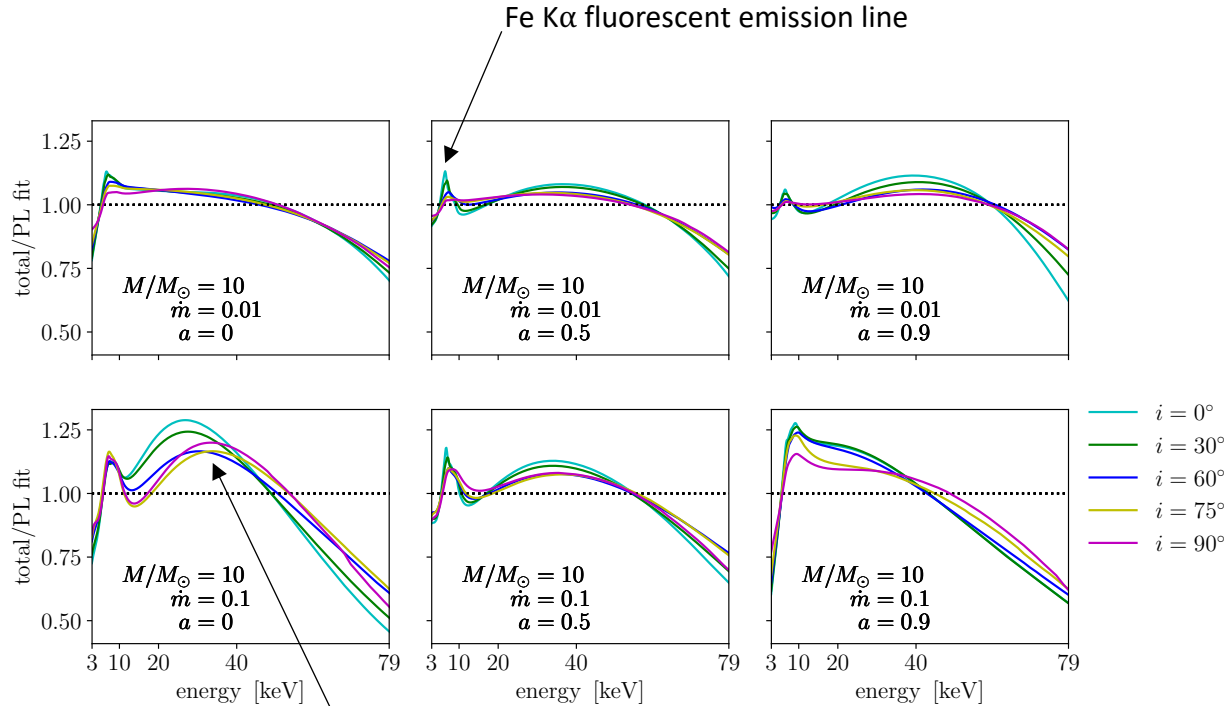
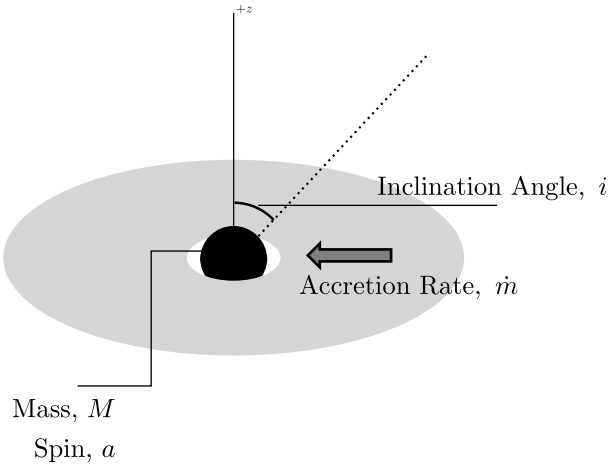
Generated X-ray spectra specifying only a *small number* of physically-meaningful parameters.



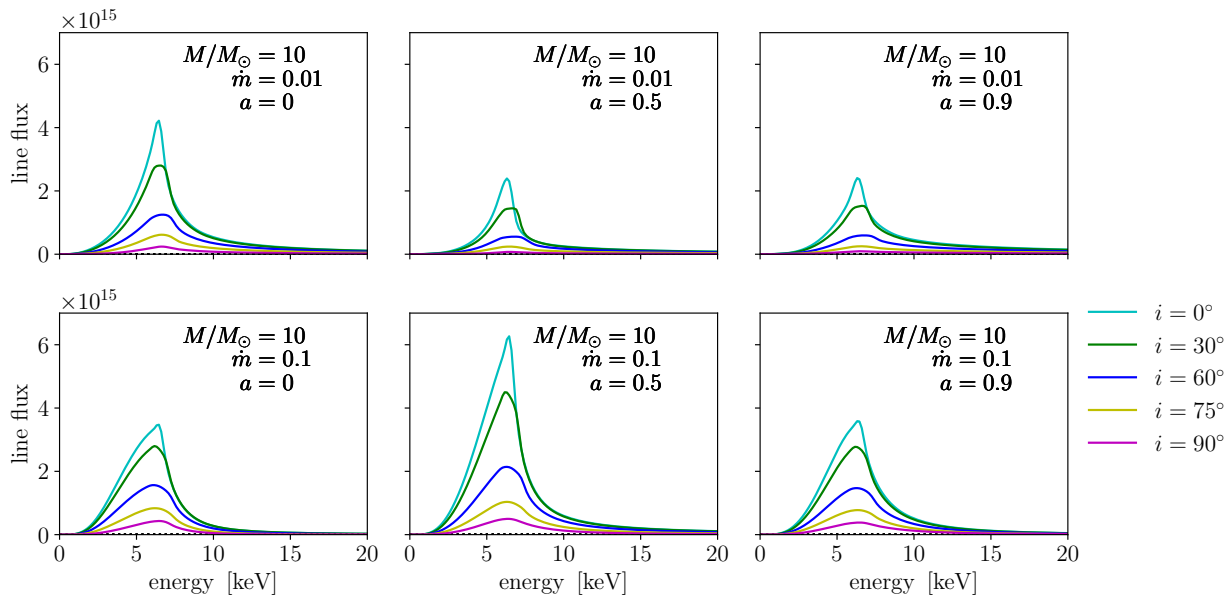
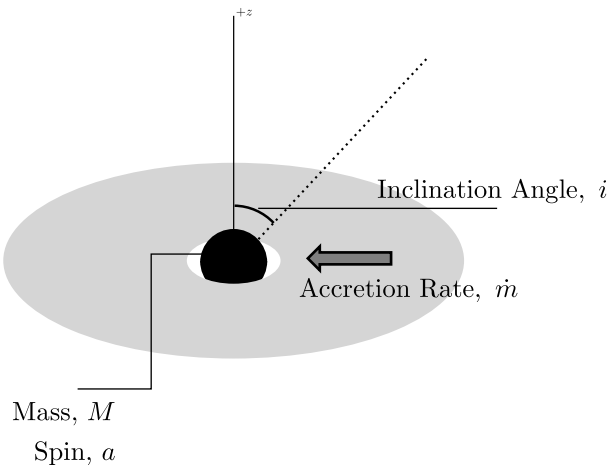
$$F_\nu/\nu \propto \nu^{-\Gamma}$$



Often useful to look at spectrum
divided by power-law fit.

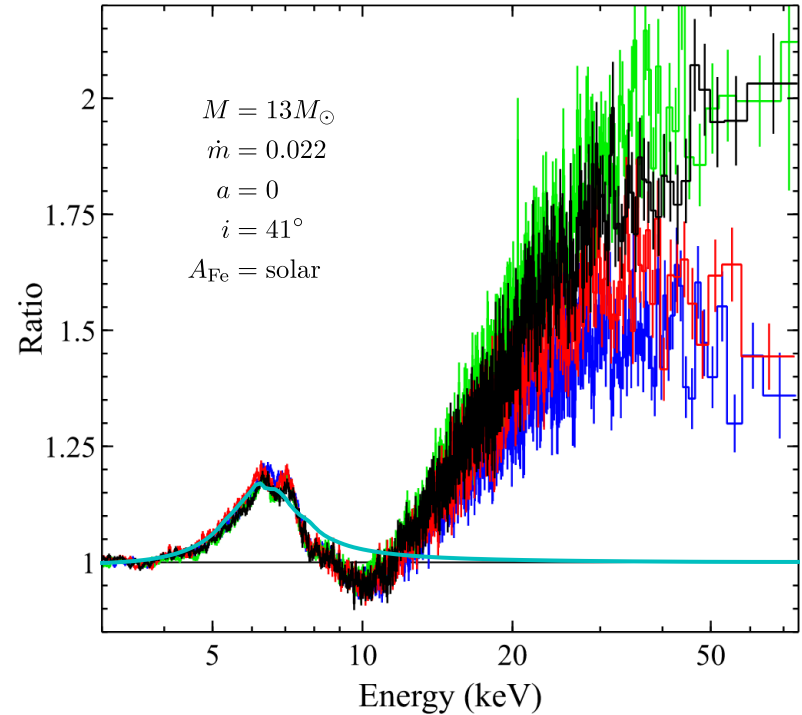
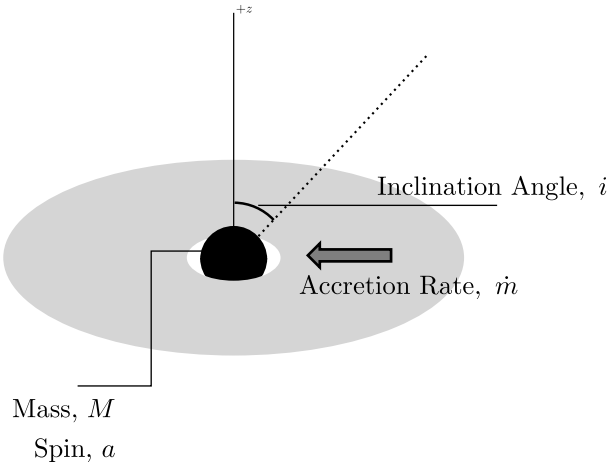


Just the Fe K α line flux (continuum-subtracted):



Our cutting edge:

Try to achieve reasonably good fits to real X-ray data.

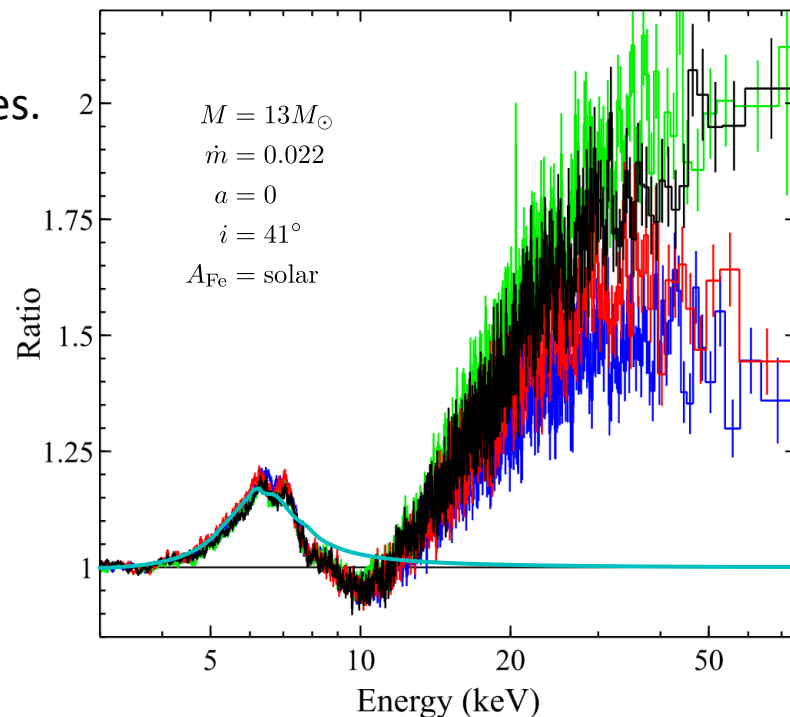


Fe K α line profile of Cyg X-1
(Walton et al. 2016).



Simulation-Derived X-Ray Spectra Highlights:

- We get strong $K\alpha$ lines with *only* solar abundances.
- Thermal peaks in the right spot, power-laws with expected slopes, roll-overs at high energy.

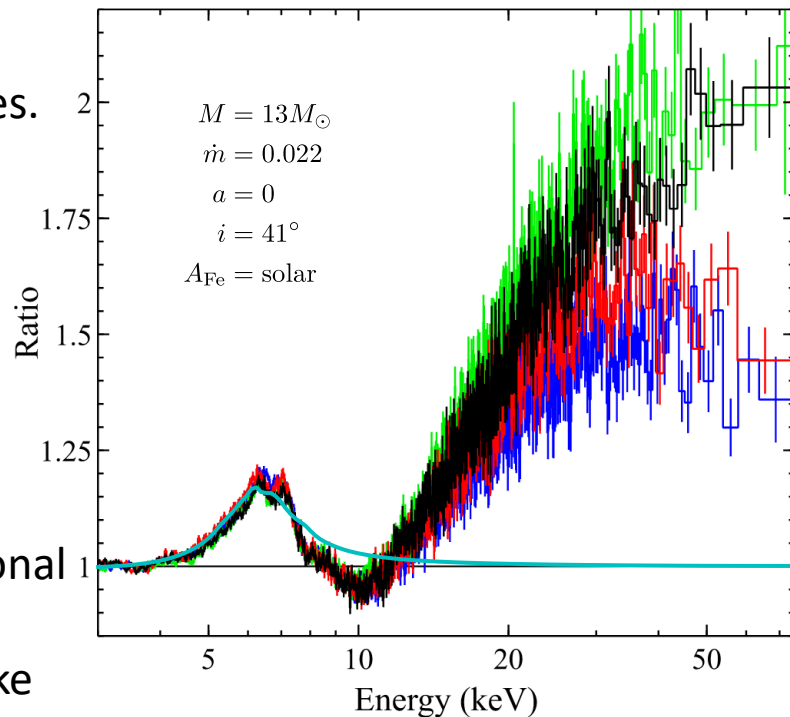


Fe $K\alpha$ line profile of Cyg X-1 overlaid with **our model**
(Walton et al. 2016).



Simulation-Derived X-Ray Spectra Highlights *and Challenges:*

- We get strong $K\alpha$ lines with *only* solar abundances.
- Thermal peaks in the right spot, power-laws with expected slopes, roll-overs at high energy.
- We do not get Compton humps *as strong* as are typically observed – could be reflection by cold, distant gas (not in our model)?
- Right now, each synthetic spectrum is fabulously expensive to compute compared to more traditional methods.
- Need to connect with seasoned observers to make more progress fitting real data.



Fe $K\alpha$ line profile of Cyg X-1 overlaid with **our model**
(Walton et al. 2016).

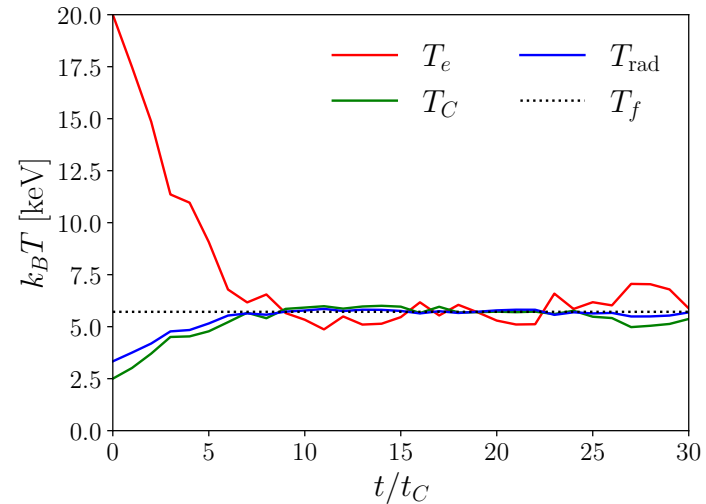


Changing gears...



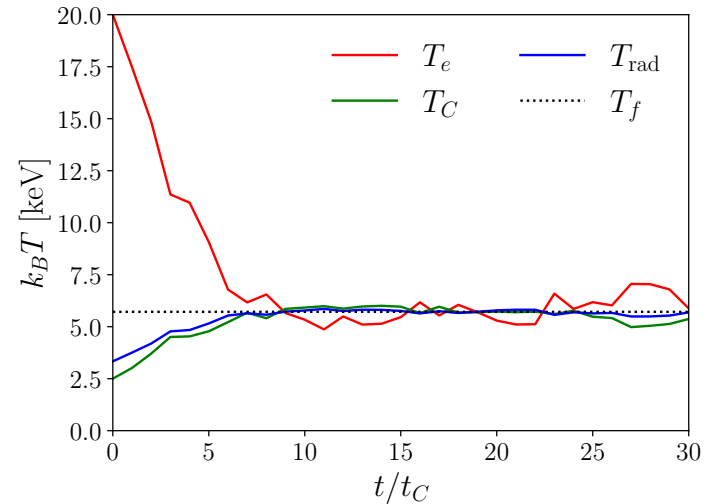
Operator Split Method for Compton Scattering in Monte Carlo Transport:

- In optically thin regimes where Compton scattering events are rare (e.g., the evacuated jet cone of a black hole simulation), *explicit* treatment of Compton scattering can lead to unacceptably variable temperature evolution.
- Example:
One zone model with only Compton.
Initially monochromatic radiation field equilibrates with thermal electron gas.



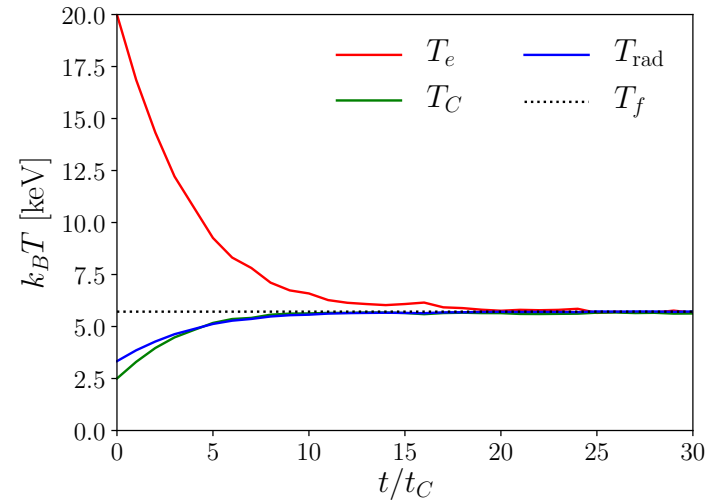
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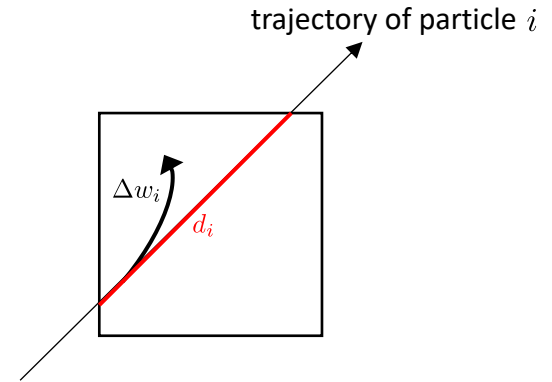
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Operator Split Method for Compton Scattering in Monte Carlo Transport:

- Instead: Track the “scattered-out” energy-weight of each particle over every flight in each cell:

$$\Delta w_i = w_{i,0} \{1 - \exp[-n_e \sigma(\nu_i, T_e) d_i]\}$$



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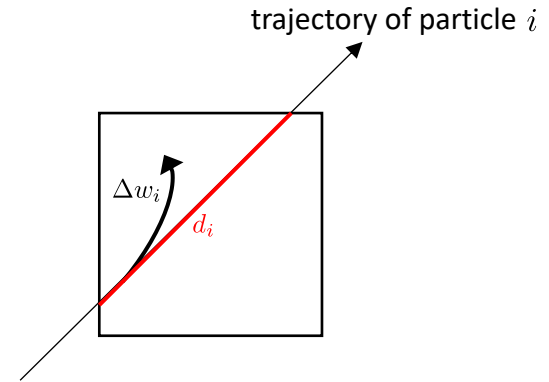
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- Re-emit new particles at the end of the time step, one per group. For the j^{th} group, emit particle with energy-weight and frequency $w_j, \langle \nu_j \rangle$ according to:

$$N_j = \int_{\nu_j^l}^{\nu_j^u} n(\nu) d\nu = \sum_i \frac{\Delta w_i}{\nu_i} \int_{\nu_j^l}^{\nu_j^u} R(\nu_i \rightarrow \nu, 1, T_e) d\nu$$

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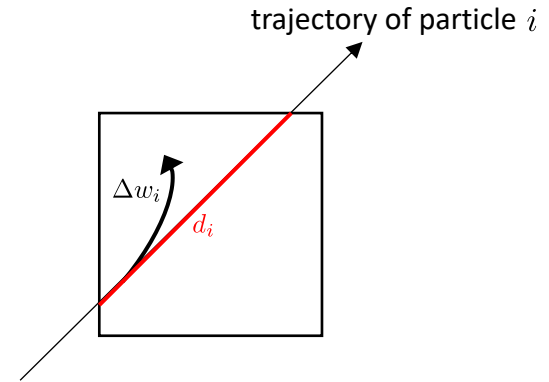
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That is:

new particle has frequency equal to the *mean frequency* of all photons scattered to group j, and represents the *number* of photons scattered to group j

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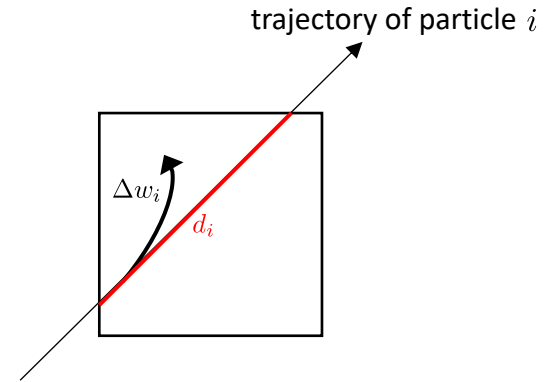
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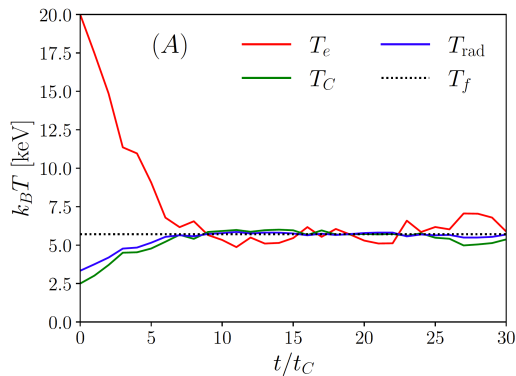


Manifestly conserves photon number.

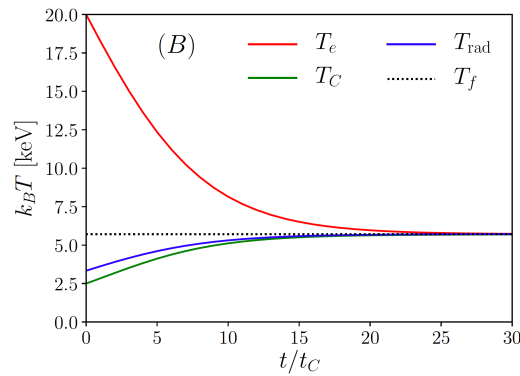
But does require integrals over the *single-scatter redistribution function*.

Operator Split Method for Compton Scattering in Monte Carlo Transport:

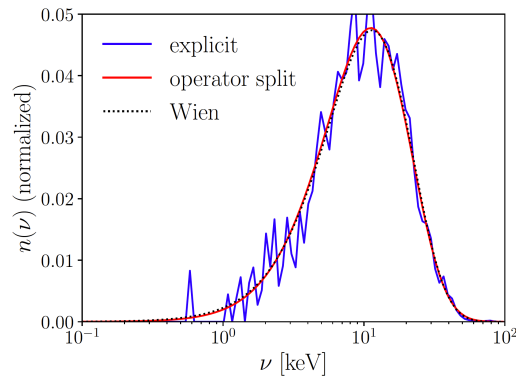
explicit
Compton



operator split
method



Temperature evolution is smoother
(and energy-conserving); also correctly
reproduces the no-induced-scattering
distribution (Wien).



Operator Split Method for Compton Scattering in Monte Carlo Transport:

- In the nonrelativistic limit $\nu, k_B T_e \ll m_e c^2$
a Gaussian approximation to the single-scatter kernel allows analytic evaluation of previous integrals:

$$R(\nu_i \rightarrow \nu') = \frac{1}{\sigma_i \sqrt{\pi}} \exp \left[-(\nu' - \mu_i)^2 / \sigma_i^2 \right]$$

$$\mu_i = \nu_i (1 + 4\Theta_e - \epsilon_i),$$

$$\sigma_i = \nu_i \sqrt{2\Theta_e + \frac{2}{5}\epsilon_i^2},$$



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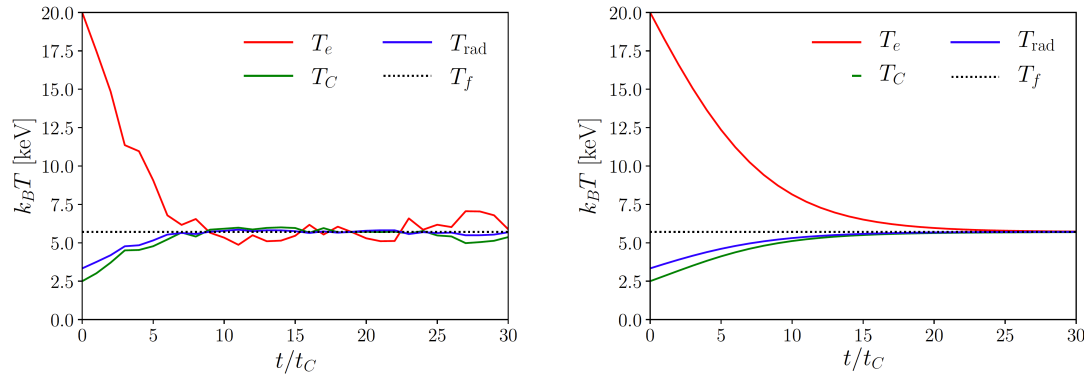
$$x_{ij}^u = \frac{\nu_j^u - \mu_i}{\sigma_i}, \quad x_{ij}^l = \frac{\nu_j^l - \mu_i}{\sigma_i}$$

In relativistic limit **compy** works – and integral values can be tabulated in advance – but still requires table-lookup.



Operator Split Method for Compton Scattering in Monte Carlo Transport:

- Limitation: If the time step is long or comparable to the mean free time between scatters, this method will *under-calculate* the Compton heating/cooling rates.

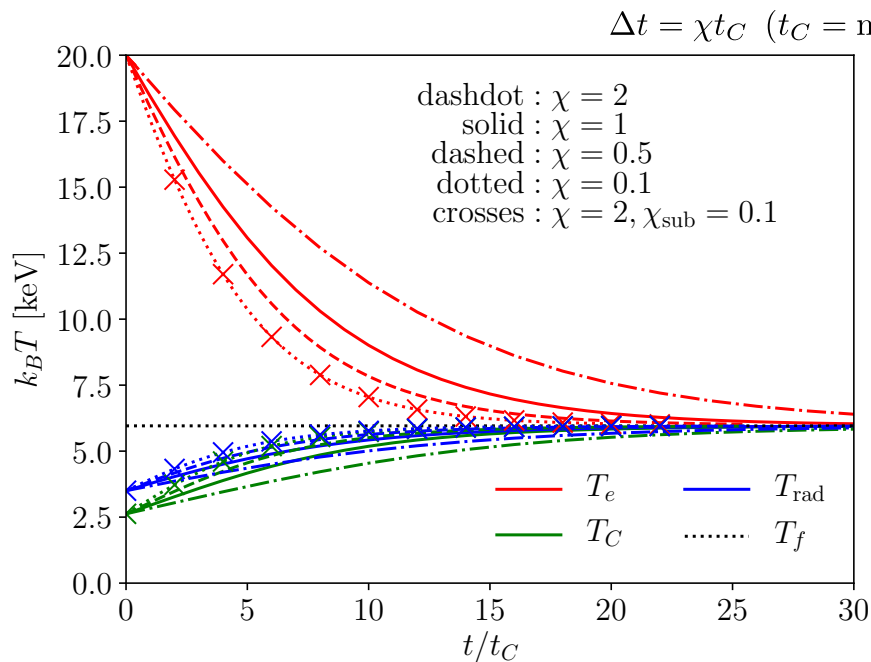


Time step equal to the mean free time between scatters.
Result: operator split run equilibrates too slowly.



Operator Split Method for Compton Scattering in Monte Carlo Transport:

- One solution is to *subcycle*:

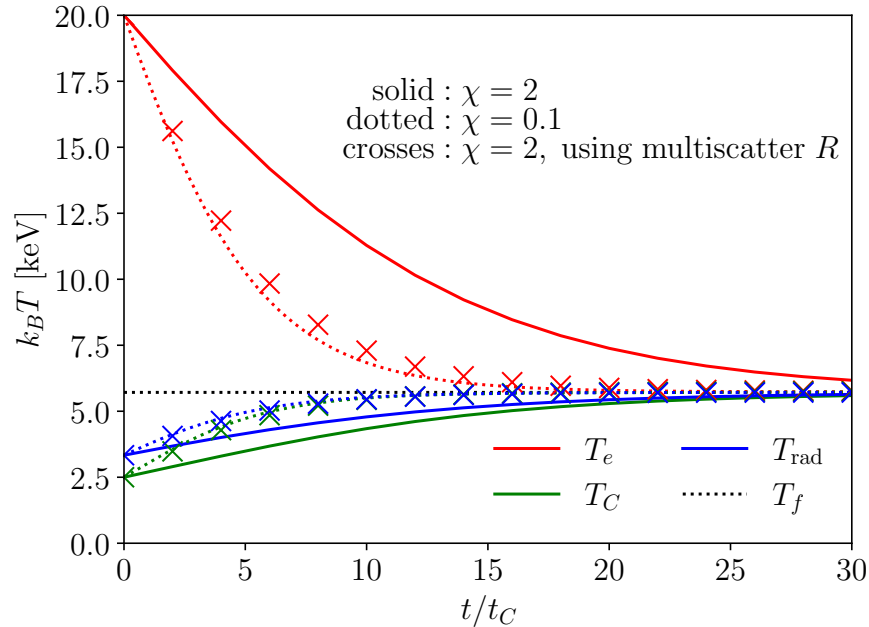


Simply run the whole procedure many times per “global” time step, emitting appropriately-averaged particles at the very end.



Operator Split Method for Compton Scattering in Monte Carlo Transport:

- A more elegant solution is to use the *multiscatter* redistribution function instead.



$$R(\nu' \rightarrow \nu, \Delta t/t_C, T_e) = \sum_{k=1}^{\infty} p(k, \Delta t/t_C) R(\nu' \rightarrow \nu, k, T_e)$$

$$p(k, \Delta t/t_C) = \frac{1}{k!} (\Delta t/t_C)^k \frac{\exp(-\Delta t/t_C)}{1 - \exp(-\Delta t/t_C)}$$

Sum over k -scatter redistribution functions to make a time-interval-dependent redistribution function.

No known multiscatter generalization of the Gaussian approximation technique – but tabulation of integral quantities in advance still possible.



Operator Split Method for Compton Scattering in Monte Carlo Transport:

- Highlights:
 - Much smoother temperature evolution.
 - Conserves photon number and energy.
 - In nonrelativistic, short time step limit, we have an inexpensive analytic formula.
 - Potentially expensive table-lookup, but much can be tabulated in advance.
 - Works just as well at relativistic temperatures – any rejection sampling inefficiency is wrapped up in the table construction in `compy`.



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 - Works just as well at relativistic temperatures – any rejection sampling inefficiency is wrapped up in the table construction in `compy`.
- Precautions:
 - Analogous to absorption/re-emission, and likewise introduces “teleportation error.”
 - Increases particle count every time step (but in a predictable way); standard population control techniques should handle this.



BACKUP SLIDES



General Relativistic Magnetohydrodynamics (GRMHD)

$$\frac{1}{\sqrt{-g}} \partial_\mu (\sqrt{-g} \rho u^\mu) = 0 \quad \text{conservation of mass}$$

density

four-velocity



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(**properties of the metric** – they don't evolve in a static spacetime)



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stress-energy tensor



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$\nu = 1$ time and 3 space coordinates

stress-energy tensor



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internal energy

fluid pressure

magnetic pressure

magnetic field 4-vector



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↑
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$$p = (\Gamma - 1)u \quad \text{ideal gas equation of state (for closure)}$$

adiabatic index



Optically thin thermal compton

- power law by multiple scattering of thermal electrons
- Number of photons $dN/dE dE = E dN/dE d\text{Log } E = f(\varepsilon) d\log \varepsilon \propto \varepsilon^{-\alpha}$
- For $\tau < 1$ scatter τ photons each time to energy $\varepsilon_{\text{out}} = (1 + 4\Theta + 16\Theta^2)\varepsilon_{\text{in}}$
- index $\alpha = \log(\text{prob}) / \log(\text{energy boost}) \sim -\log \tau / \log(1 + 4\Theta + 16\Theta^2)$

courtesy of
Chris Done

